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Measurement of transverse energy–energy correlations in multi-jet events in pp collisions at $\sqrt{s} = 7$ TeV using the ATLAS detector and determination of the strong coupling constant $\alpha_s(m_Z)$

ATLAS Collaboration^{*}

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ABSTRACT

High transverse momentum jets produced in pp collisions at a centre of mass energy of 7 TeV are used to measure the transverse energy–energy correlation function and its associated azimuthal asymmetry. The data were recorded with the ATLAS detector at the LHC in the year 2011 and correspond to an integrated luminosity of 158 pb^{-1} . The selection criteria demand the average transverse momentum of the two leading jets in an event to be larger than 250 GeV. The data at detector level are well described by Monte Carlo event generators. They are unfolded to the particle level and compared with theoretical calculations at next-to-leading-order accuracy. The agreement between data and theory is good and provides a precision test of perturbative Quantum Chromodynamics at large momentum transfers. From this comparison, the strong coupling constant given at the Z boson mass is determined to be $\alpha_s(m_Z) = 0.1173 \pm 0.0010$ (exp.) $^{+0.0065}_{-0.0026}$ (theo.).

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1. Introduction

The study of jet production at the LHC provides a quantitative test of Quantum Chromodynamics, QCD, at the highest momentum transfers. Theoretical calculations for jet cross-sections in hadronic collisions have been carried out up to next-to-leading order (NLO) accuracy in the strong coupling constant α_s [1–3] and extensively compared with the data [4–10]. These calculations are valid for configurations with up to four jets in the final state.

Event shape variables have been measured in all major e^+e^- experiments, as well as in experiments at the electron–proton collider HERA. These studies were recently extended to hadron colliders with measurements of the transverse thrust and the transverse minor [11,12] at the Tevatron [13] and the LHC [14,15].

Energy–energy correlations (EEC), i.e. measurements of the energy-weighted angular distributions of hadron pairs produced in e^+e^- annihilation, were proposed in Refs. [16,17] as an alternative event shape variable not based on the determination of the thrust principal axis [18] or the sphericity tensor [19]. The EEC function and its asymmetry, AEEC, were subsequently calculated in $\mathcal{O}(\alpha_s^2)$ [20–22], and their measurements [23–35] have had significant impact on the precision tests of perturbative QCD and in the determination of the strong coupling constant in e^+e^- annihilation experiments; a recent review is given in Ref. [36]. The EEC are

by construction not affected by soft divergences, and as a consequence of this they are calculable at high orders.

The transverse energy–energy correlation function, TEEC, and its asymmetry, ATEEC, were proposed as the analogous variables at hadron collider experiments in Ref. [37], where predictions to leading order (LO) were also presented. The NLO corrections were calculated recently in Ref. [38] using NLOJET++ [2,3]. These calculations allow for a numerical determination of the NLO predictions for the TEEC and ATEEC, i.e. the coefficients of the second order polynomials in the strong coupling constant. They are used in this paper for quantitative precision tests of QCD including a determination of the strong coupling constant. The TEEC is defined as:

$$\frac{1}{\sigma} \frac{d\Sigma}{d(\cos\phi)} = \frac{1}{\sigma} \sum_{ij} \int \frac{d\sigma}{dx_{Ti} dx_{Tj} d(\cos\phi)} x_{Ti} x_{Tj} dx_{Ti} dx_{Tj}, \quad (1)$$

where the sum runs over all pairs of jets in the final state with azimuthal¹ angular difference $\phi = \Delta\varphi_{ij}$ and $x_{Ti} = E_{Ti}/E_T$ is the transverse energy carried by jet i in units of the sum of jet transverse energies $E_T = \sum_i E_{Ti}$. In order to cancel uncertainties that

¹ ATLAS uses a right-handed coordinate system with its origin at the nominal interaction point (IP) in the centre of the detector and the z -axis along the beam pipe. The x -axis points from the IP to the centre of the LHC ring, and the y -axis points upward. Cylindrical coordinates (r, φ) are used in the transverse plane, φ being the azimuthal angle around the beam pipe. The pseudorapidity is defined in terms of the polar angle θ as $\eta = -\ln \tan(\theta/2)$.

^{*} E-mail address: atlas_publications@cern.ch.

are constant over $\cos\phi \in [-1, 1]$, it is useful to define the azimuthal asymmetry of the TEEC (ATEEC) as

$$\frac{1}{\sigma} \frac{d\Sigma^{\text{asym}}}{d(\cos\phi)} \equiv \frac{1}{\sigma} \frac{d\Sigma}{d(\cos\phi)} \Big|_{\phi} - \frac{1}{\sigma} \frac{d\Sigma}{d(\cos\phi)} \Big|_{\pi-\phi}. \quad (2)$$

This Letter presents a measurement of the TEEC and its associated asymmetry using high-energy jets.

2. The ATLAS detector

The ATLAS detector [39] is a multi-purpose particle physics detector with a forward–backward symmetric cylindrical geometry and a solid angle coverage of almost 4π .

The inner tracking system covers the pseudorapidity range $|\eta| < 2.5$, and consists of a silicon pixel detector, a silicon microstrip detector, and, for $|\eta| < 2.0$, a transition radiation tracker. It is surrounded by a thin superconducting solenoid providing a 2 T magnetic field along the beam direction. A high-granularity liquid-argon sampling electromagnetic calorimeter covers the region $|\eta| < 3.2$. An iron/scintillator tile hadronic calorimeter provides coverage in the range $|\eta| < 1.7$. The endcap and forward regions, spanning $1.5 < |\eta| < 4.9$, are instrumented with liquid-argon calorimeters for electromagnetic and hadronic measurements. The muon spectrometer surrounds the calorimeters. It consists of three large air-core superconducting toroid systems and separate trigger and high-precision tracking chambers providing accurate muon tracking for $|\eta| < 2.7$.

The trigger system [40] has three consecutive levels: level 1 (L1), level 2 (L2) and the event filter (EF). The L1 triggers are hardware-based and use coarse detector information to identify regions of interest, whereas the L2 triggers are software-based and perform a fast online data reconstruction. Finally, the EF uses reconstruction algorithms similar to the offline versions with the full detector granularity.

3. Monte Carlo samples

Multi-jet production in pp collisions is represented by the convolution of the production cross-sections for parton–parton scattering with the parton distribution functions. Monte Carlo (MC) generators differ in the approximations used to calculate the underlying short-distance QCD process, in the way parton showers are built to take into account higher-order effects and in the fragmentation scheme responsible for long-distance effects. For this analysis, two different MC approaches are used, depending on whether the underlying hard process is considered to be $2 \rightarrow 2$ or multi-legged. The generated events are then processed with the ATLAS full detector simulation [41] based on GEANT4 [42].

The baseline MC samples are generated using PYTHIA 6.423 [43] with the matrix elements for the underlying $2 \rightarrow 2$ processes calculated at LO using the MRST2007LO* parton distribution functions (PDF) [44] and matched to transverse-momentum-ordered parton showers. The AUET2B tune [45,46] is used to model the underlying event (UE) and the hadronisation follows the Lund string model [47].

Additional samples are generated with HERWIG++ 2.5.1 [48], using the CTEQ6.6 PDF [49] and the UE7000 tune for the underlying event [50]. HERWIG++ uses angular-ordered parton showers, a cluster hadronisation scheme and its own underlying-event parameterisation given by JIMMY [51].

A different approach to simulate multi-jet final states is followed by ALPGEN [52]. This approach is based on LO matrix-element calculations for $2 \rightarrow n$ multi-parton final states, with $n \leq 6$, interfaced with HERWIG+JIMMY [53,51] to provide the parton shower, hadronisation and underlying-event models. ALPGEN is

known to provide a good description of the multi-jet final states as measured by ATLAS [54].

4. Event selection and jet calibration

The data used in this analysis were recorded in 2011 at $\sqrt{s} = 7$ TeV and collected using a single-jet trigger. It requires at least one jet, reconstructed with the anti- k_t algorithm [55] with radius parameter $R = 0.4$ as implemented in FASTJET [56]. The jet transverse energy, $E_T = E \sin\theta$, is required to be greater than 135 GeV at the trigger level. This trigger is fully efficient at reconstructed transverse energies above 240 GeV. Taking into account the prescale factor of this trigger, the data collected correspond to an effective integrated luminosity of $\mathcal{L}_{\text{eff}} = 158 \text{ pb}^{-1}$ [57].

Events are required to have at least one primary vertex, with five or more associated tracks with transverse momentum $p_T > 400$ MeV. If there is more than one primary vertex, the vertex maximising $\sum p_T^2$ is chosen. MC simulated events are subject to a reweighting algorithm in order to match the average number of interactions per bunch-crossing observed in the data.

In the analysis, jets are reconstructed with the same algorithm as used in the trigger, the anti- k_t algorithm with radius parameter $R = 0.4$. The input objects to the jet algorithm are topological clusters of energy deposits in the calorimeters [58]. The baseline calibration for these clusters corrects their energy using local hadronic calibration [59,60]. The four-momentum of an uncalibrated jet is defined as the sum of the four-momenta of its constituent clusters, which are considered massless. The resulting jets are massive. However, the effect of this mass is marginal for jets in the kinematic range considered in this paper.

The jet calibration procedure includes energy corrections for multiple pp interactions in the same or neighbouring bunch crossings, termed “pileup” in the following, as well as angular corrections to ensure that the jet originates from the primary vertex. Effects due to energy losses in inactive material, shower leakage, the magnetic field, as well as inefficiencies in energy clustering and jet reconstruction, are taken into account. This is done using an MC-based correction, in bins of η and p_T , derived from the relation of the reconstructed jet energy to the energy of the corresponding hadron-level jet, not including muons or non-interacting particles. In a final step, an in situ calibration corrects for residual differences in the jet response between the MC simulation and the data using momentum-balance techniques for dijet, $\gamma + \text{jet}$, $Z + \text{jet}$ and multi-jet final states. This so-called jet energy scale (JES) [61] is subject to uncertainties including those affecting the energy of well-measured objects, like Z bosons and photons. The total JES uncertainty is given by a set of independent sources, correlated in p_T . The uncertainty in the p_T of individual jets due to the JES increases from (1–4)% for $|\eta| < 1.8$, to 5% for $1.8 < |\eta| < 4.5$.

The selected events must have at least two jets with transverse momentum $p_T > 50$ GeV and pseudorapidity $|\eta| < 2.5$. The two leading jets are further required to fulfil $p_{T1} + p_{T2} > 500$ GeV. In addition, jets are required to satisfy quality criteria that reject beam-induced backgrounds [62], as well as criteria for the fraction of the momentum of tracks within the jet which arise from the primary interaction vertex. The number of selected events in data is 3.8×10^5 , with an average jet multiplicity $\langle N_{\text{jet}} \rangle = 2.6$. The resulting distribution for $(p_{T1} + p_{T2})/2$ extends up to 1.3 TeV with an average value of 305 GeV.

5. Results at the detector level

The selected events are used to measure the TEEC and its associated asymmetry ATEEC, as defined in Equations (1) and (2). The

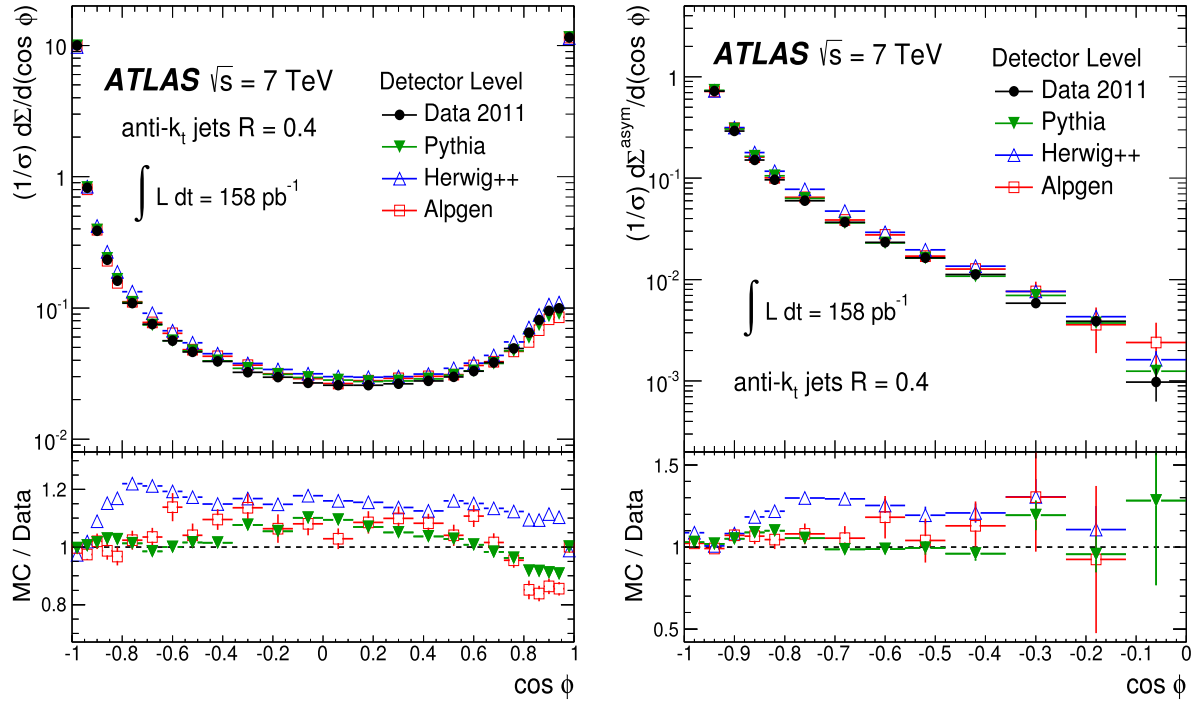


Fig. 1. The detector-level distributions for the transverse energy–energy correlation TEEC (left) and its asymmetry ATEEC (right) along with comparisons to MC model expectations. The uncertainties shown are statistical only. The first bin of the ATEEC distribution has a negative value and is therefore not included in the figure.

TEEC distribution for a sample of N events is obtained by calculating the cosines of the angles in the transverse plane between all possible pairs of jets in each event. Every pair (i, j) represents an entry in the distribution, which is then weighted with the normalised product of the transverse energies. The weights w_{ij} are defined as

$$w_{ij} = x_{Ti}x_{Tj} = \frac{E_{Ti}E_{Tj}}{(\sum_k E_{Tk})^2}, \quad (3)$$

such that for a given event their sum is always unity, as the self correlations $i = j$ are also taken into account. The resulting distribution is then divided by the number of events, which normalises it to unit area. This weighting procedure reduces the sensitivity to the jet energy scale and resolution.

Fig. 1 shows the TEEC and ATEEC distributions along with comparisons to detector-level PYTHIA, HERWIG and ALPGEN expectations. The TEEC exhibits peaks at $\cos \phi = 1$ (self correlations) and near $\cos \phi = -1$, with a rather flat central region around $\cos \phi = 0$. These features are similar to those observed in e^+e^- annihilation, as described in Ref. [31]. The central region is expected to be dominated by hard radiation processes while multiple soft radiation is expected to be important in the $\cos \phi \simeq \pm 1$ regions.

The description of the TEEC is good in the back-to-back region $\cos \phi \simeq -1$ for both PYTHIA 6 and ALPGEN. Differences up to 10% are observed in the central part, while the region of small angles shows differences as large as about 15%. The description by HERWIG++ is poorer. The ATEEC exhibits a steep fall-off, which is reproduced by both PYTHIA 6 and ALPGEN. HERWIG++ shows some discrepancies as large as 30%.

6. Correction to particle level

The data are corrected to the particle level in order to take into account detector efficiencies and resolutions. This allows a direct comparison with theoretical calculations, as well as with measurements of other experiments.

Particle-level jets are reconstructed in MC events using all particles with average lifetime $\tau > 10^{-11}$ s, including muons and neutrinos. The kinematic selection criteria are the same as for the detector-level distribution. The unfolding relies on a bin-by-bin correction given by the ratios of the particle-level to detector-level distributions in the PYTHIA AUET2B sample, which is then applied to the detector-level distributions in data. To check the effect of bin migrations on the unfolding procedure, an iterative Bayesian method [63] as implemented in RooUNFOLD [64] is also used. The convergence criteria is fulfilled when the linear sum over all bins of the absolute relative differences from one iteration to the next drops below 10^{-2} . The method converges after five iterations. The differences between the two approaches are negligible, compared to the statistical uncertainties, in the full range of $\cos \phi$. This is expected due to the high azimuthal resolution of the jet axis, which is 10 mrad.

The following experimental sources of uncertainty are considered for this measurement:

- **Jet energy scale:** The uncertainty due to the jet energy scale (JES) [61] is calculated using MC techniques by varying each jet energy and momentum by one standard deviation for each of the 63 independent sources of the JES uncertainty, and propagated to the TEEC. These uncertainties depend on the jet transverse momentum and pseudorapidity. The total uncertainty due to the JES is calculated as the sum in quadrature of all independent uncertainties. In order to investigate the effect of possible correlations between JES sources in the analysis, two alternative scenarios with weaker and stronger correlations have been considered [61]. The impact of the change of correlation configurations, as well as of the number of JES independent sources, on the value of $\alpha_s(m_Z)$ and its experimental error is found to be negligible. The values of the JES uncertainty are typically asymmetric for both the TEEC and ATEEC distributions, although the values for

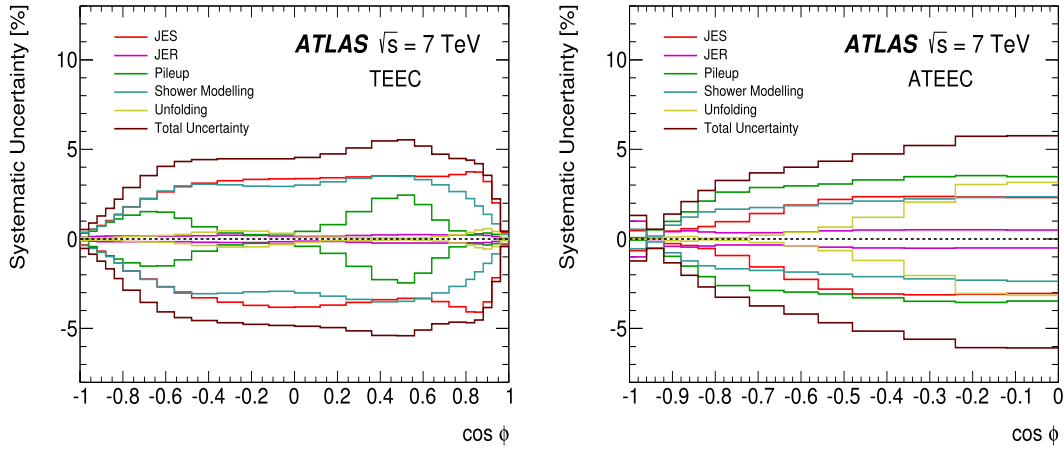


Fig. 2. Relative systematic uncertainties for the TEEC (left) and the ATEEC (right) as a function of $\cos \phi$.

this asymmetry are small. Thus, the positive and negative parts of the uncertainty are independently summed in quadrature. The TEEC distribution has a total uncertainty of up to 3.5% from the JES sources, the largest contributions being due to close-by jets and to the different response to jets initiated by gluons or quarks. This is the dominant experimental systematic uncertainty in the analysis.

- **Jet energy resolution:** The uncertainty in the jet energy resolution [65] is propagated to the TEEC by smearing each jet transverse momentum by a p_T - and η -dependent factor accounting for the resolution uncertainty. The size of this uncertainty is below 1% for both the TEEC and the ATEEC distributions.
- **Pileup:** The pileup uncertainty is estimated by comparing the ratio of the detector-level TEEC and ATEEC distributions obtained in samples with reduced ($\mu < 6$) and enhanced pileup activity ($\mu > 6$). Here μ is the average number of interactions per bunch crossing [57]. These ratios are formed in both data and MC simulation and the difference is assigned as the pileup systematic uncertainty, which is as large as 2% (4%) for the TEEC (ATEEC). The size of this dedicated estimate is larger than what is predicted by the sum of the two sources of uncertainty due to pileup included in the JES uncertainty. The envelope of the two different estimates is used.
- **Parton shower modelling:** To estimate the uncertainty due to the parton shower modelling, the data unfolded with PYTHIA 6 and HERWIG++ are compared. The parton shower and hadronisation models in the two generators are different, as is the implementation of UE effects. The size of this uncertainty is as large as 3.5% (2.5%) for the TEEC (ATEEC).
- **Unfolding:** To estimate the uncertainty associated with the unfolding procedure, a data-driven method is used to test its stability. This method relies on the reweighting of the particle-level projection of the unfolding transfer matrix so that the agreement between the detector-level projection and the data is enhanced. This modified detector-level distribution is then unfolded using the correction factors described above. The difference between the modified particle-level distribution and the nominal one is then taken as the uncertainty. This uncertainty is smaller than 0.5% for the full $\cos \phi$ range.

Other possible sources of uncertainty are also studied, such as the jet angular resolution and jet quality selection procedure. They are found to be at the per mille level, much smaller than the statistical uncertainty on the corrected data, and are therefore neglected. To reduce the effect of statistical fluctuations, all the independent systematic uncertainties discussed here are smoothed separately.

Fig. 2 shows the breakdown of the systematic uncertainties for both the TEEC and the ATEEC, together with the total, obtained as the sum in quadrature of every independent source discussed above.

The TEEC and ATEEC distributions, once corrected for detector effects, are shown in Fig. 3, together with their total uncertainties, while numerical values are given in Tables 1 and 2.

As already seen in the detector-level distributions, PYTHIA 6 and ALPGEN give a fair description of the data both for the TEEC and ATEEC. The back-to-back region $\cos \phi \sim -1$ is well described, while small discrepancies, at the level of 10%, are observed in the central region of the TEEC and for large $\cos \phi$ values. The description by HERWIG++ is poorer.

The shape of the ATEEC is very similar to that observed at e^+e^- colliders, see Refs. [23–35], and well reproduced by PYTHIA 6 and ALPGEN.

7. Theoretical predictions and uncertainties

In perturbative QCD (pQCD), according to the factorisation theorem [66], final-state observables can be expressed as a convolution of the partonic cross-sections, $\hat{\sigma}$, with the parton distribution functions. Thus, in this particular case, the TEEC distribution to leading order in the strong coupling constant, can be expressed as the three-jet, energy-weighted, differential cross-section in $\cos \phi$, normalised to the integrated two-jet cross-section. This can be schematically expressed as

$$\frac{1}{\sigma} \frac{d\Sigma}{d(\cos \phi)} = \frac{\Sigma_{a_i, b_i} f_{a_1}(x_1) f_{a_2}(x_2) \otimes \hat{\Sigma}^{a_1 a_2 \rightarrow b_1 b_2 b_3}}{\Sigma_{a_i, b_i} f_{a_1}(x_1) f_{a_2}(x_2) \otimes \hat{\sigma}^{a_1 a_2 \rightarrow b_1 b_2}}, \quad (4)$$

where $\hat{\Sigma}^{a_1 a_2 \rightarrow b_1 b_2 b_3}$ is the transverse energy–energy weighted partonic cross-section, x_i ($i = 1, 2$) are the fractional longitudinal momenta of the initial-state partons, $f_{a_1}(x_1)$ and $f_{a_2}(x_2)$ are the PDF, and \otimes denotes a convolution over the appropriate variables. The denominator of Eq. (4) is the integrated dijet cross-section used to normalise the TEEC.

The pQCD NLO calculations of the TEEC and ATEEC distributions are performed using NLOJET++ [23] interfaced with the MSTW 2008 [67], CT10 [68], NNPDF 2.3 [69] and HERAPDF 1.5 [70] parton distribution functions at NNLO. Typically, $\mathcal{O}(10^{10})$ events are generated for these calculations. This involves the calculation of the $2 \rightarrow 3$ partonic subprocesses at NLO accuracy and of the $2 \rightarrow 4$ partonic subprocesses at tree level. In order to avoid the double collinear singularities appearing in the latter [38], the angular range is restricted to $|\cos \phi| < 0.92$.

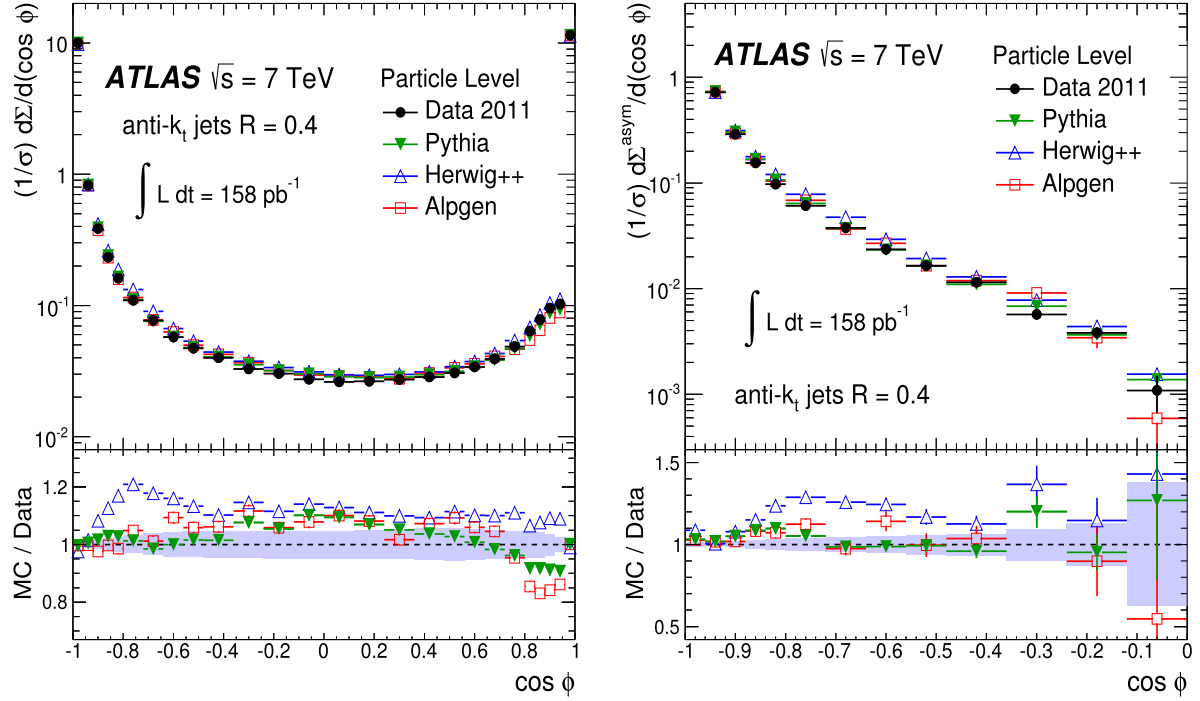


Fig. 3. The unfolded distributions for transverse energy–energy correlation (left) and its asymmetry (right) along with comparisons to MC expectations. The statistical uncertainties are shown with error bars, while the total experimental uncertainties are shown in a shaded band.

Table 1

Values of the transverse energy–energy correlation function (TEEC). The statistical and systematic uncertainties, due to Jet Energy Scale and Resolution (JES and JER), shower modelling as well as pileup and unfolding, are shown in the subsequent columns. Uncertainties marked with a dash (–) are smaller than 0.00005.

| $\cos \phi$ | TEEC | Stat. | JES | JER | Shower | Pileup | Unfolding |
|----------------|--------|--------|--------------------|--------|--------|--------|-----------|
| (–1.00, –0.96) | 10.008 | 0.008 | +0.033 –0.034 | 0.009 | 0.037 | 0.008 | 0.008 |
| (–0.96, –0.92) | 0.8218 | 0.0047 | +0.0044 –0.0040 | 0.0011 | 0.0044 | 0.0036 | 0.0005 |
| (–0.92, –0.88) | 0.3848 | 0.0029 | +0.0029 –0.0026 | 0.0006 | 0.0028 | 0.0028 | 0.0002 |
| (–0.88, –0.84) | 0.2324 | 0.0022 | +0.0024 –0.0022 | 0.0004 | 0.0023 | 0.0022 | 0.0001 |
| (–0.84, –0.80) | 0.1612 | 0.0017 | +0.0022 –0.0022 | 0.0003 | 0.0022 | 0.0018 | 0.0002 |
| (–0.80, –0.72) | 0.1095 | 0.0009 | +0.0020 –0.0020 | 0.0002 | 0.0020 | 0.0015 | 0.0002 |
| (–0.72, –0.64) | 0.0767 | 0.0008 | +0.0017 –0.0017 | 0.0001 | 0.0017 | 0.0012 | 0.0001 |
| (–0.64, –0.56) | 0.0574 | 0.0006 | +0.0015 –0.0015 | 0.0001 | 0.0015 | 0.0009 | 0.0001 |
| (–0.56, –0.48) | 0.0472 | 0.0005 | +0.0014 –0.0014 | 0.0001 | 0.0014 | 0.0005 | 0.0001 |
| (–0.48, –0.36) | 0.0400 | 0.0004 | +0.0012 –0.0013 | 0.0001 | 0.0012 | 0.0003 | 0.0001 |
| (–0.36, –0.24) | 0.0329 | 0.0004 | +0.0011 –0.0012 | 0.0001 | 0.0010 | 0.0001 | 0.0001 |
| (–0.24, –0.12) | 0.0302 | 0.0003 | +0.0010 –0.0011 | 0.0001 | 0.0009 | 0.0001 | 0.0001 |
| (–0.12, 0.00) | 0.0273 | 0.0003 | +0.0009 –0.0010 | – | 0.0008 | 0.0001 | 0.0001 |
| (0.00, 0.12) | 0.0262 | 0.0003 | +0.0009 –0.0010 | – | 0.0008 | 0.0001 | – |
| (0.12, 0.24) | 0.0264 | 0.0003 | +0.0009 –0.0010 | – | 0.0008 | 0.0002 | – |
| (0.24, 0.36) | 0.0272 | 0.0003 | +0.0009 –0.0010 | 0.0001 | 0.0009 | 0.0004 | – |
| (0.36, 0.48) | 0.0286 | 0.0003 | +0.0010 –0.0010 | 0.0001 | 0.0010 | 0.0006 | – |
| (0.48, 0.56) | 0.0306 | 0.0004 | +0.0011 –0.0010 | 0.0001 | 0.0011 | 0.0008 | – |
| (0.56, 0.64) | 0.0340 | 0.0004 | +0.0012 –0.0011 | 0.0001 | 0.0011 | 0.0006 | – |
| (0.64, 0.72) | 0.0391 | 0.0004 | +0.0014 –0.0014 | 0.0001 | 0.0012 | 0.0004 | 0.0001 |
| (0.72, 0.80) | 0.0487 | 0.0004 | +0.0017 –0.0018 | 0.0001 | 0.0013 | 0.0002 | 0.0001 |
| (0.80, 0.84) | 0.0639 | 0.0007 | +0.0024 –0.0026 | 0.0001 | 0.0014 | 0.0002 | 0.0002 |
| (0.84, 0.88) | 0.0780 | 0.0008 | +0.0029 –0.0032 | 0.0002 | 0.0014 | 0.0002 | 0.0004 |
| (0.88, 0.92) | 0.0955 | 0.0009 | +0.0031 –0.0033 | 0.0002 | 0.0013 | 0.0003 | 0.0005 |
| (0.92, 0.96) | 0.1025 | 0.0009 | +0.0021 –0.0022 | 0.0001 | 0.0009 | 0.0003 | 0.0004 |
| (0.96, 1.00) | 11.448 | 0.003 | +0.039 –0.036 | 0.006 | 0.030 | 0.008 | 0.008 |

Table 2

Values of the asymmetry on the transverse energy–energy correlation function (ATEEC). The statistical and systematic uncertainties, due to Jet Energy Scale and Resolution (JES and JER), shower modelling as well as pileup and unfolding, are shown in the subsequent columns. Uncertainties marked with a dash (–) are smaller than 0.00005.

| $\cos\phi$ | ATEEC | Stat. | JES | JER | Shower | Pileup | Unfolding |
|----------------|---------|--------|--------------------|--------|--------|--------|-----------|
| (–1.00, –0.96) | –1.4406 | 0.0083 | +0.0094 –0.0066 | 0.0144 | 0.0078 | 0.0010 | 0.0001 |
| (–0.96, –0.92) | 0.7193 | 0.0048 | +0.0002 –0.0000 | 0.0002 | 0.0012 | 0.0037 | 0.0001 |
| (–0.92, –0.88) | 0.2893 | 0.0030 | +0.0012 –0.0008 | 0.0012 | 0.0022 | 0.0028 | 0.0003 |
| (–0.88, –0.84) | 0.1544 | 0.0023 | +0.0009 –0.0006 | 0.0007 | 0.0019 | 0.0023 | 0.0002 |
| (–0.84, –0.80) | 0.0973 | 0.0019 | +0.0007 –0.0005 | 0.0004 | 0.0015 | 0.0020 | – |
| (–0.80, –0.72) | 0.0608 | 0.0010 | +0.0006 –0.0006 | 0.0002 | 0.0010 | 0.0016 | – |
| (–0.72, –0.64) | 0.0376 | 0.0009 | +0.0005 –0.0006 | 0.0001 | 0.0007 | 0.0011 | 0.0001 |
| (–0.64, –0.56) | 0.0235 | 0.0007 | +0.0004 –0.0005 | 0.0001 | 0.0004 | 0.0007 | 0.0001 |
| (–0.56, –0.48) | 0.0165 | 0.0007 | +0.0004 –0.0005 | 0.0001 | 0.0003 | 0.0005 | 0.0001 |
| (–0.48, –0.36) | 0.0115 | 0.0005 | +0.0003 –0.0004 | 0.0001 | 0.0002 | 0.0004 | 0.0001 |
| (–0.36, –0.24) | 0.0057 | 0.0004 | +0.0001 –0.0002 | – | 0.0001 | 0.0002 | 0.0001 |
| (–0.24, –0.12) | 0.0038 | 0.0004 | +0.0001 –0.0001 | – | 0.0001 | 0.0001 | 0.0001 |
| (–0.12, 0.00) | 0.0011 | 0.0004 | – | – | – | – | – |

The renormalisation and factorisation scales, inherent in any pQCD calculation, are usually taken to reflect the typical transverse momentum of the process under investigation. For the TEEC and ATEEC calculations, they are taken to be

$$\mu_R = \mu_F = \frac{p_{T1} + p_{T2}}{2}, \quad (5)$$

where p_{T1} and p_{T2} are the transverse momenta of the two leading jets. This is also the choice in Ref. [71]. The value of the strong coupling constant at a given scale is connected to $\alpha_s(m_Z)$ using the two-loop beta function [2,3].

The NLO theoretical predictions are subsequently corrected for non-perturbative effects such as hadronisation and the underlying event. This correction is calculated using the leading-logarithm parton shower generators PYTHIA 6 and HERWIG++ interfaced with different tunes. The full MC generator particle-level predictions with these effects switched on are compared with the parton-level predictions before hadronisation and without UE effects. From this comparison a bin-by-bin correction factor is calculated as the ratio of the two predictions, which is then used to correct the NLOJET++ output. They are found to deviate from unity by about 1% for both PYTHIA 6 and HERWIG++ for most of the $|\cos\phi| < 0.92$ range.

Three main theoretical uncertainties are considered for the analysis: those corresponding to the renormalisation and factorisation scale variations, those corresponding to the PDF, and those on the non-perturbative corrections.

- **Scale uncertainty:** The ambiguity in the choice of the renormalisation and factorisation scales gives rise to a scale uncertainty. To estimate it, the scales μ_R and μ_F are varied by a factor of two up and down, with the additional requirement that $0.5 \leq \mu_R/\mu_F \leq 2$. From all those variations, the largest uncertainty is obtained when both μ_R and μ_F are varied simultaneously by the same factor from the nominal scale. These two combinations are used to define the envelope of the scale uncertainty for both the TEEC and ATEEC. The size of the scale uncertainty is highly asymmetric and is at most about 8% for the TEEC distribution, and somewhat smaller for the ATEEC.
- **PDF uncertainty:** The CT10 parton distribution functions provide 50 variations for the 25 fitted parameters at the 90% confidence level. Each of the 25 parameters are varied up and down following the CT10 recommendations in Ref. [68], and are combined for each bin of the TEEC and ATEEC distributions following the prescription given in Ref. [72]. The size of

the PDF uncertainty, once scaled at 68% confidence level, is about 1.5%. A similar procedure is used for the MSTW2008, NNPDF 2.3 and HERAPDF 1.5 parton distribution functions.

- **Uncertainties in the non-perturbative corrections:** The non-perturbative corrections (NPC) are calculated using PYTHIA 6 interfaced to the AUET2B and AMBT2B tunes [45,46], as well as HERWIG++ with the UE7000 tune [50]. Moreover, PYTHIA 8 interfaced to the 4C and AU2 tunes is also used. An uncertainty is derived by considering, on a bin-by-bin basis, the maximum difference between the nominal PYTHIA AUET2B and any other tune. Its size is below 1% for most of the angular range considered.

8. Determination of the strong coupling $\alpha_s(m_Z)$

The evaluation of $\alpha_s(m_Z)$ is made by minimising a χ^2 function taking into account correlations between the systematic uncertainties using nuisance parameters λ_k , one for each source of uncertainty. These nuisance parameters are normalised to zero mean and unit variance. The minimum of the χ^2 function is found in a 66-dimensional space, one dimension corresponding to $\alpha_s(m_Z)$ and the rest to the nuisance parameters associated with the experimental errors. The function to be minimised is defined as

$$\chi^2(\alpha_s, \vec{\lambda}) = \sum_i \frac{(x_i - F_i(\alpha_s, \vec{\lambda}))^2}{\Delta x_i^2 + \Delta \tau_i^2} + \sum_k \lambda_k^2, \quad (6)$$

where the NLOJET++ predictions are varied according to

$$F_i(\alpha_s, \vec{\lambda}) = \psi_i(\alpha_s) \left(1 + \sum_k \lambda_k \sigma_k^{(i)} \right). \quad (7)$$

In these expressions, x_i corresponds to the data points in each distribution (TEEC or ATEEC), and Δx_i are their statistical uncertainties. $\Delta \tau_i$ are the statistical errors on the NLOJET++ predictions, while $\sigma_k^{(i)}$ correspond to the k -th source of experimental uncertainty in the bin i .

The functions $\psi_i(\alpha_s)$ are analytical expressions parameterising the dependence of each observable (TEEC or ATEEC) on the strong coupling constant. They are obtained by fitting the predictions for each bin as a function of $\alpha_s(m_Z)$. This function is chosen to be a parabola, as the theoretical predictions account for terms quadratic in α_s . The quality of the fit to the NLO theoretical predictions is found to be excellent for each bin of the TEEC and ATEEC. The uncertainties from these fits are negligible.

Table 3

Results for α_s from fits to the TEEC function using different PDF sets, namely MSTW 2008, CT10, NNPDF 2.3 and HERAPDF 1.5, together with experimental as well as theoretical uncertainties due to scale and PDF choices and non-perturbative corrections.

| PDF | $\alpha_s(m_Z)$ value | χ^2/N_{dof} |
|-------------|---|-------------------------|
| MSTW 2008 | 0.1175 ± 0.0010 (exp.) $^{+0.0059}_{-0.0019}$ (scale) ± 0.0006 (PDF) ± 0.0002 (NPC) | 29.0/21 |
| CT10 | 0.1173 ± 0.0010 (exp.) $^{+0.0063}_{-0.0020}$ (scale) ± 0.0017 (PDF) ± 0.0002 (NPC) | 28.4/21 |
| NNPDF 2.3 | 0.1183 ± 0.0010 (exp.) $^{+0.0059}_{-0.0013}$ (scale) ± 0.0009 (PDF) ± 0.0002 (NPC) | 29.3/21 |
| HERAPDF 1.5 | 0.1167 ± 0.0007 (exp.) $^{+0.0040}_{-0.0008}$ (scale) $^{+0.0007}_{-0.0024}$ (PDF) ± 0.0001 (NPC) | 28.7/21 |

Table 4

Results for α_s from fits to the ATEEC function using different PDF sets, namely MSTW 2008, CT10, NNPDF 2.3 and HERAPDF 1.5, together with experimental as well as theoretical uncertainties due to scale and PDF choices. The uncertainty due to the non-perturbative corrections is negligible.

| PDF | $\alpha_s(m_Z)$ value | χ^2/N_{dof} |
|-------------|--|-------------------------|
| MSTW 2008 | 0.1195 ± 0.0017 (exp.) $^{+0.0055}_{-0.0015}$ (scale) ± 0.0006 (PDF) | 12.7/10 |
| CT10 | 0.1195 ± 0.0018 (exp.) $^{+0.0060}_{-0.0015}$ (scale) ± 0.0016 (PDF) | 12.6/10 |
| NNPDF 2.3 | 0.1206 ± 0.0018 (exp.) $^{+0.0057}_{-0.0013}$ (scale) ± 0.0009 (PDF) | 12.2/10 |
| HERAPDF 1.5 | 0.1182 ± 0.0013 (exp.) $^{+0.0041}_{-0.0008}$ (scale) $^{+0.0007}_{-0.0025}$ (PDF) | 12.1/10 |

The theoretical uncertainties on the predictions are treated by varying the theoretical distributions by each independent source of uncertainty (scale, all independent PDF uncertainties and non-perturbative corrections) and repeating the fit using the modified theoretical input.

The fit to the TEEC data exhibits shifts in a few nuisance parameters, which are always compatible with the $\pm 1\sigma$ band. The results for the strong coupling constant obtained using different parameterisations of the PDF are summarised in Table 3, together with the experimental uncertainties and the values of χ^2/N_{dof} .

The final value for the TEEC fits is chosen to be the one obtained using CT10, since its PDF uncertainty is largest and serves as an envelope covering the variations with different PDF sets as shown in Table 3:

$$\alpha_s(m_Z) = 0.1173 \pm 0.0010 \text{ (exp.) } ^{+0.0063}_{-0.0020} \text{ (scale)} \pm 0.0017 \text{ (PDF)} \pm 0.0002 \text{ (NPC)}. \quad (8)$$

The fit to the ATEEC data does not show any significant shift in the values of the nuisance parameters. In this case, the fit results in the values for the strong coupling constant which are summarised in Table 4.

The final value for the ATEEC fit is also chosen to be the one obtained using the CT10 parton distribution functions:

$$\alpha_s(m_Z) = 0.1195 \pm 0.0018 \text{ (exp.) } ^{+0.0060}_{-0.0015} \text{ (scale)} \pm 0.0016 \text{ (PDF)}. \quad (9)$$

The agreement between the fitted theoretical NLO predictions, including non-perturbative corrections, and the data is good as shown in Fig. 4 and indicated by the χ^2 values given in Tables 3 and 4. Restricting the angular region in the fits to $(-0.72, 0.72)$, yield values of the strong coupling constant which vary within experimental uncertainties. The values of $\alpha_s(m_Z)$ found in this analysis are in agreement with the world average $\alpha_s(m_Z) = 0.1185 \pm 0.0006$ [73], as well as with other determinations of the strong coupling constant from the data collected at the LHC [71,10,74].

Calculations beyond NLO accuracy, which are already available for processes such as top-quark pair [75] or Higgs boson production [76], are needed for multi-jet production at LHC energies. They are expected to reduce the scale uncertainties, which are the limiting factor in this determination of the strong coupling constant.

9. Summary

First measurements of the TEEC and ATEEC functions are presented using 158 pb^{-1} of pp collision data at 7 TeV recorded by the ATLAS experiment at the LHC. For this purpose, multi-jet final states are selected requiring jets, reconstructed with the anti- k_t algorithm and radius parameter $R = 0.4$, with $p_T > 50 \text{ GeV}$ and $|\eta| < 2.5$ and such that the scalar sum of the transverse momenta of the two leading jets is above 500 GeV. The TEEC and ATEEC data are fairly well described by PYTHIA 6 and ALPGEN, while the HERWIG++ MC simulation shows some discrepancies which can be as large as 30%.

The TEEC and the ATEEC at the particle level are compared to perturbative QCD predictions at NLO accuracy. The renormalisation and factorisation scales are chosen to be $(p_{T1} + p_{T2})/2$, ranging from 250 to 1300 GeV and with an average value of 305 GeV. Through their construction, both the TEEC and ATEEC functions are less affected by experimental effects such as the jet energy scale and resolution or pileup than absolute cross-section measurements. Similarly, the PDF uncertainties in their theoretical predictions, as given by Eq. (4), cancel to a large extent. This renders these observables well suited to determine the strong coupling constant. The data for $|\cos\phi| < 0.92$ are fitted to the QCD predictions obtained with NLOJET++ to determine the value of the strong coupling constant. For the TEEC, which provides the experimentally more accurate determination, the result of the fit using the CT10 PDF yields

$$\alpha_s(m_Z) = 0.1173 \pm 0.0010 \text{ (exp.) } ^{+0.0063}_{-0.0020} \text{ (scale)} \pm 0.0017 \text{ (PDF)} \pm 0.0002 \text{ (NPC)}. \quad (10)$$

The present determination of $\alpha_s(m_Z)$ is limited by the uncertainties due to the choice of renormalisation and factorisation scales.

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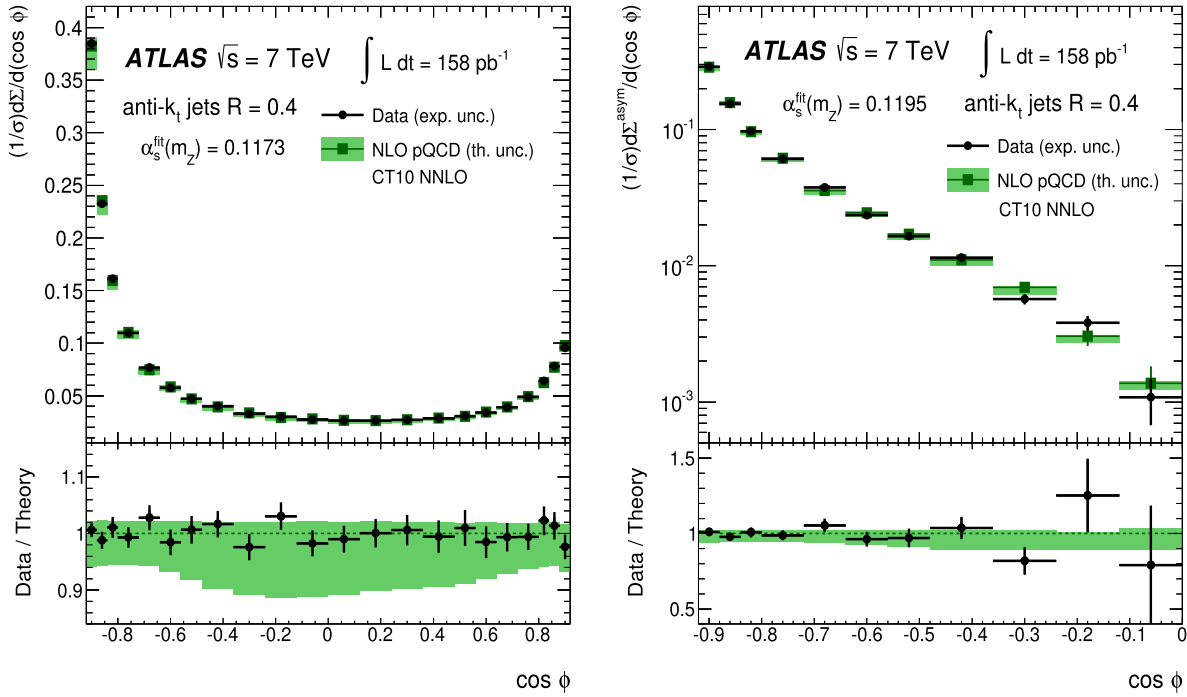


Fig. 4. The unfolded distributions for transverse energy-energy correlation (left) and its asymmetry (right) compared with the results of a fit to pQCD NLO calculations including non-perturbative corrections. The green shaded band indicates the uncertainty on the theoretical predictions, which includes the sum in quadrature of uncertainties associated with scale, α_s , PDF and NPC. The statistical uncertainties on the predictions are indicated by green error bars, appreciable only on the tail of the ATEEC. The solid error bars on the data points (in black) indicate the experimental uncertainties taking into account the correlations between them. The fitted values of the strong coupling constant are $\alpha_s^{\text{fit}}(m_Z) = 0.1173$ (TEEC) and $\alpha_s^{\text{fit}}(m_Z) = 0.1195$ (ATEEC). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

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ATLAS Collaboration

G. Aad⁸⁵, B. Abbott¹¹³, J. Abdallah¹⁵¹, O. Abidinov¹¹, R. Aben¹⁰⁷, M. Abolins⁹⁰, O.S. AbouZeid¹⁵⁸, H. Abramowicz¹⁵³, H. Abreu¹⁵², R. Abreu¹¹⁶, Y. Abulaiti^{146a,146b}, B.S. Acharya^{164a,164b,a}, L. Adamczyk^{38a}, D.L. Adams²⁵, J. Adelman¹⁰⁸, S. Adomeit¹⁰⁰, T. Adye¹³¹, A.A. Affolder⁷⁴, T. Agatonovic-Jovin¹³, J. Agricola⁵⁴, J.A. Aguilar-Saavedra^{126a,126f}, S.P. Ahlen²², F. Ahmadov^{65,b},

G. Aielli ^{133a,133b}, H. Akerstedt ^{146a,146b}, T.P.A. Åkesson ⁸¹, A.V. Akimov ⁹⁶, G.L. Alberghi ^{20a,20b}, J. Albert ¹⁶⁹, S. Albrand ⁵⁵, M.J. Alconada Verzini ⁷¹, M. Aleksa ³⁰, I.N. Aleksandrov ⁶⁵, C. Alexa ^{26a}, G. Alexander ¹⁵³, T. Alexopoulos ¹⁰, M. Alhroob ¹¹³, G. Alimonti ^{91a}, L. Alio ⁸⁵, J. Alison ³¹, S.P. Alkire ³⁵, B.M.M. Allbrooke ¹⁴⁹, P.P. Allport ⁷⁴, A. Aloisio ^{104a,104b}, A. Alonso ³⁶, F. Alonso ⁷¹, C. Alpigiani ⁷⁶, A. Althimer ³⁵, B. Alvarez Gonzalez ³⁰, D. Álvarez Piqueras ¹⁶⁷, M.G. Alviggi ^{104a,104b}, B.T. Amadio ¹⁵, K. Amako ⁶⁶, Y. Amaral Coutinho ^{24a}, C. Amelung ²³, D. Amidei ⁸⁹, S.P. Amor Dos Santos ^{126a,126c}, A. Amorim ^{126a,126b}, S. Amoroso ⁴⁸, N. Amram ¹⁵³, G. Amundsen ²³, C. Anastopoulos ¹³⁹, L.S. Ancu ⁴⁹, N. Andari ¹⁰⁸, T. Andeen ³⁵, C.F. Anders ^{58b}, G. Anders ³⁰, J.K. Anders ⁷⁴, K.J. Anderson ³¹, A. Andreazza ^{91a,91b}, V. Andrei ^{58a}, S. Angelidakis ⁹, I. Angelozzi ¹⁰⁷, P. Anger ⁴⁴, A. Angerami ³⁵, F. Anghinolfi ³⁰, A.V. Anisenkov ^{109,c}, N. Anjos ¹², A. Annovi ^{124a,124b}, M. Antonelli ⁴⁷, A. Antonov ⁹⁸, J. Antos ^{144b}, F. Anulli ^{132a}, M. Aoki ⁶⁶, L. Aperio Bella ¹⁸, G. Arabidze ⁹⁰, Y. Arai ⁶⁶, J.P. Araque ^{126a}, A.T.H. Arce ⁴⁵, F.A. Arduh ⁷¹, J.-F. Arguin ⁹⁵, S. Argyropoulos ⁶³, M. Arik ^{19a}, A.J. Armbruster ³⁰, O. Arnaez ³⁰, V. Arnal ⁸², H. Arnold ⁴⁸, M. Arratia ²⁸, O. Arslan ²¹, A. Artamonov ⁹⁷, G. Artoni ²³, S. Asai ¹⁵⁵, N. Asbah ⁴², A. Ashkenazi ¹⁵³, B. Åsman ^{146a,146b}, L. Asquith ¹⁴⁹, K. Assamagan ²⁵, R. Astalos ^{144a}, M. Atkinson ¹⁶⁵, N.B. Atlay ¹⁴¹, K. Augsten ¹²⁸, M. Auresseu ^{145b}, G. Avolio ³⁰, B. Axen ¹⁵, M.K. Ayoub ¹¹⁷, G. Azuelos ^{95,d}, M.A. Baak ³⁰, A.E. Baas ^{58a}, M.J. Baca ¹⁸, C. Bacci ^{134a,134b}, H. Bachacou ¹³⁶, K. Bachas ¹⁵⁴, M. Backes ³⁰, M. Backhaus ³⁰, P. Bagiachi ^{132a,132b}, P. Bagnaia ^{132a,132b}, Y. Bai ^{33a}, T. Bain ³⁵, J.T. Baines ¹³¹, O.K. Baker ¹⁷⁶, E.M. Baldin ^{109,c}, P. Balek ¹²⁹, T. Balestri ¹⁴⁸, F. Balli ⁸⁴, E. Banas ³⁹, Sw. Banerjee ¹⁷³, A.A.E. Bannoura ¹⁷⁵, H.S. Bansil ¹⁸, L. Barak ³⁰, E.L. Barberio ⁸⁸, D. Barberis ^{50a,50b}, M. Barbero ⁸⁵, T. Barillari ¹⁰¹, M. Barisonzi ^{164a,164b}, T. Barklow ¹⁴³, N. Barlow ²⁸, S.L. Barnes ⁸⁴, B.M. Barnett ¹³¹, R.M. Barnett ¹⁵, Z. Barnovska ⁵, A. Baroncelli ^{134a}, G. Barone ²³, A.J. Barr ¹²⁰, F. Barreiro ⁸², J. Barreiro Guimarães da Costa ⁵⁷, R. Bartoldus ¹⁴³, A.E. Barton ⁷², P. Bartos ^{144a}, A. Basalaev ¹²³, A. Bassalat ¹¹⁷, A. Basye ¹⁶⁵, R.L. Bates ⁵³, S.J. Batista ¹⁵⁸, J.R. Batley ²⁸, M. Battaglia ¹³⁷, M. Baue ^{132a,132b}, F. Bauer ¹³⁶, H.S. Bawa ^{143,e}, J.B. Beacham ¹¹¹, M.D. Beattie ⁷², T. Beau ⁸⁰, P.H. Beauchemin ¹⁶¹, R. Beccherle ^{124a,124b}, P. Bechtel ²¹, H.P. Beck ^{17,f}, K. Becker ¹²⁰, M. Becker ⁸³, M. Beckingham ¹⁷⁰, C. Becot ¹¹⁷, A.J. Beddall ^{19b}, A. Beddall ^{19b}, V.A. Bednyakov ⁶⁵, C.P. Bee ¹⁴⁸, L.J. Beemster ¹⁰⁷, T.A. Beermann ³⁰, M. Begel ²⁵, J.K. Behr ¹²⁰, C. Belanger-Champagne ⁸⁷, W.H. Bell ⁴⁹, G. Bella ¹⁵³, L. Bellagamba ^{20a}, A. Bellerive ²⁹, M. Bellomo ⁸⁶, K. Belotskiy ⁹⁸, O. Beltramello ³⁰, O. Benary ¹⁵³, D. Benchekroun ^{135a}, M. Bender ¹⁰⁰, K. Bendtz ^{146a,146b}, N. Benekos ¹⁰, Y. Benhammou ¹⁵³, E. Benhar Nocchioli ⁴⁹, J.A. Benitez Garcia ^{159b}, D.P. Benjamin ⁴⁵, J.R. Bensinger ²³, S. Bentvelsen ¹⁰⁷, L. Beresford ¹²⁰, M. Beretta ⁴⁷, D. Berge ¹⁰⁷, E. Bergeas Kuutmann ¹⁶⁶, N. Berger ⁵, F. Berghaus ¹⁶⁹, J. Beringer ¹⁵, C. Bernard ²², N.R. Bernard ⁸⁶, C. Bernius ¹¹⁰, F.U. Bernlochner ²¹, T. Berry ⁷⁷, P. Berta ¹²⁹, C. Bertella ⁸³, G. Bertoli ^{146a,146b}, F. Bertolucci ^{124a,124b}, C. Bertsche ¹¹³, D. Bertsche ¹¹³, M.I. Besana ^{91a}, G.J. Besjes ³⁶, O. Bessidskaia Bylund ^{146a,146b}, M. Bessner ⁴², N. Besson ¹³⁶, C. Betancourt ⁴⁸, S. Bethke ¹⁰¹, A.J. Bevan ⁷⁶, W. Bhimji ¹⁵, R.M. Bianchi ¹²⁵, L. Bianchini ²³, M. Bianco ³⁰, O. Biebel ¹⁰⁰, D. Biedermann ¹⁶, S.P. Bieniek ⁷⁸, M. Biglietti ^{134a}, J. Bilbao De Mendizabal ⁴⁹, H. Bilokon ⁴⁷, M. Bindi ⁵⁴, S. Binet ¹¹⁷, A. Bingul ^{19b}, C. Bini ^{132a,132b}, S. Biondi ^{20a,20b}, C.W. Black ¹⁵⁰, J.E. Black ¹⁴³, K.M. Black ²², D. Blackburn ¹³⁸, R.E. Blair ⁶, J.-B. Blanchard ¹³⁶, J.E. Blanco ⁷⁷, T. Blazek ^{144a}, I. Bloch ⁴², C. Blocker ²³, W. Blum ^{83,*}, U. Blumenschein ⁵⁴, G.J. Bobbink ¹⁰⁷, V.S. Bobrovnikov ^{109,c}, S.S. Bocchetta ⁸¹, A. Bocci ⁴⁵, C. Bock ¹⁰⁰, M. Boehler ⁴⁸, J.A. Bogaerts ³⁰, D. Bogavac ¹³, A.G. Bogdanchikov ¹⁰⁹, C. Boehm ^{146a}, V. Boisvert ⁷⁷, T. Bold ^{38a}, V. Boldea ^{26a}, A.S. Boldyrev ⁹⁹, M. Bomben ⁸⁰, M. Bona ⁷⁶, M. Boonekamp ¹³⁶, A. Borisov ¹³⁰, G. Borissov ⁷², S. Borroni ⁴², J. Bortfeldt ¹⁰⁰, V. Bortolotto ^{60a,60b,60c}, K. Bos ¹⁰⁷, D. Boscherini ^{20a}, M. Bosman ¹², J. Boudreau ¹²⁵, J. Bouffard ², E.V. Bouhova-Thacker ⁷², D. Boumediene ³⁴, C. Bourdarios ¹¹⁷, N. Bousson ¹¹⁴, A. Boveia ³⁰, J. Boyd ³⁰, I.R. Boyko ⁶⁵, I. Bozic ¹³, J. Bracinik ¹⁸, A. Brandt ⁸, G. Brandt ⁵⁴, O. Brandt ^{58a}, U. Bratzler ¹⁵⁶, B. Brau ⁸⁶, J.E. Brau ¹¹⁶, H.M. Braun ^{175,*}, S.F. Brazzale ^{164a,164c}, W.D. Breaden Madden ⁵³, K. Brendlinger ¹²², A.J. Brennan ⁸⁸, L. Brenner ¹⁰⁷, R. Brenner ¹⁶⁶, S. Bressler ¹⁷², K. Bristow ^{145c}, T.M. Bristow ⁴⁶, D. Britton ⁵³, D. Britzger ⁴², F.M. Brochu ²⁸, I. Brock ²¹, R. Brock ⁹⁰, J. Bronner ¹⁰¹, G. Brooijmans ³⁵, T. Brooks ⁷⁷, W.K. Brooks ^{32b}, J. Brosamer ¹⁵, E. Brost ¹¹⁶, J. Brown ⁵⁵, P.A. Bruckman de Renstrom ³⁹, D. Bruncko ^{144b}, R. Bruneliere ⁴⁸, A. Bruni ^{20a}, G. Bruni ^{20a}, M. Bruschi ^{20a}, N. Bruscino ²¹, L. Bryngemark ⁸¹, T. Buanes ¹⁴, Q. Buat ¹⁴², P. Buchholz ¹⁴¹, A.G. Buckley ⁵³, S.I. Buda ^{26a}, I.A. Budagov ⁶⁵, F. Buehrer ⁴⁸, L. Bugge ¹¹⁹, M.K. Bugge ¹¹⁹, O. Bulekov ⁹⁸, D. Bullock ⁸, H. Burckhart ³⁰, S. Burdin ⁷⁴, C.D. Burgard ⁴⁸, B. Burghgrave ¹⁰⁸, S. Burke ¹³¹, I. Burmeister ⁴³, E. Busato ³⁴, D. Büscher ⁴⁸,

V. Büscher⁸³, P. Bussey⁵³, J.M. Butler²², A.I. Butt³, C.M. Buttar⁵³, J.M. Butterworth⁷⁸, P. Butti¹⁰⁷, W. Buttinger²⁵, A. Buzatu⁵³, A.R. Buzykaev^{109,c}, S. Cabrera Urbán¹⁶⁷, D. Caforio¹²⁸, V.M. Cairo^{37a,37b}, O. Cakir^{4a}, N. Calace⁴⁹, P. Calafiura¹⁵, A. Calandri¹³⁶, G. Calderini⁸⁰, P. Calfayan¹⁰⁰, L.P. Caloba^{24a}, D. Calvet³⁴, S. Calvet³⁴, R. Camacho Toro³¹, S. Camarda⁴², P. Camarri^{133a,133b}, D. Cameron¹¹⁹, R. Caminal Armadans¹⁶⁵, S. Campana³⁰, M. Campanelli⁷⁸, A. Campoverde¹⁴⁸, V. Canale^{104a,104b}, A. Canepa^{159a}, M. Cano Bret^{33e}, J. Cantero⁸², R. Cantrill^{126a}, T. Cao⁴⁰, M.D.M. Capeans Garrido³⁰, I. Caprini^{26a}, M. Caprini^{26a}, M. Capua^{37a,37b}, R. Caputo⁸³, R. Cardarelli^{133a}, F. Cardillo⁴⁸, T. Carli³⁰, G. Carlino^{104a}, L. Carminati^{91a,91b}, S. Caron¹⁰⁶, E. Carquin^{32a}, G.D. Carrillo-Montoya³⁰, J.R. Carter²⁸, J. Carvalho^{126a,126c}, D. Casadei⁷⁸, M.P. Casado¹², M. Casolino¹², E. Castaneda-Miranda^{145a}, A. Castelli¹⁰⁷, V. Castillo Gimenez¹⁶⁷, N.F. Castro^{126a,g}, P. Catastini⁵⁷, A. Catinaccio³⁰, J.R. Catmore¹¹⁹, A. Cattai³⁰, J. Caudron⁸³, V. Cavaliere¹⁶⁵, D. Cavalli^{91a}, M. Cavalli-Sforza¹², V. Cavasinni^{124a,124b}, F. Ceradini^{134a,134b}, B.C. Cerio⁴⁵, K. Cerny¹²⁹, A.S. Cerqueira^{24b}, A. Cerri¹⁴⁹, L. Cerrito⁷⁶, F. Cerutti¹⁵, M. Cerv³⁰, A. Cervelli¹⁷, S.A. Cetin^{19c}, A. Chafaq^{135a}, D. Chakraborty¹⁰⁸, I. Chalupkova¹²⁹, P. Chang¹⁶⁵, J.D. Chapman²⁸, D.G. Charlton¹⁸, C.C. Chau¹⁵⁸, C.A. Chavez Barajas¹⁴⁹, S. Cheatham¹⁵², A. Chegwidden⁹⁰, S. Chekanov⁶, S.V. Chekulaev^{159a}, G.A. Chelkov^{65,h}, M.A. Chelstowska⁸⁹, C. Chen⁶⁴, H. Chen²⁵, K. Chen¹⁴⁸, L. Chen^{33d,i}, S. Chen^{33c}, X. Chen^{33f}, Y. Chen⁶⁷, H.C. Cheng⁸⁹, Y. Cheng³¹, A. Cheplakov⁶⁵, E. Cheremushkina¹³⁰, R. Cherkaoui El Moursli^{135e}, V. Chernyatin^{25,*}, E. Cheu⁷, L. Chevalier¹³⁶, V. Chiarella⁴⁷, G. Chiarelli^{124a,124b}, G. Chiodini^{73a}, A.S. Chisholm¹⁸, R.T. Chislett⁷⁸, A. Chitan^{26a}, M.V. Chizhov⁶⁵, K. Choi⁶¹, S. Chouridou⁹, B.K.B. Chow¹⁰⁰, V. Christodoulou⁷⁸, D. Chromek-Burckhart³⁰, J. Chudoba¹²⁷, A.J. Chuinard⁸⁷, J.J. Chwastowski³⁹, L. Chytka¹¹⁵, G. Ciapetti^{132a,132b}, A.K. Ciftci^{4a}, D. Cinca⁵³, V. Cindro⁷⁵, I.A. Cioara²¹, A. Ciocio¹⁵, F. Ciotto^{104a,104b}, Z.H. Citron¹⁷², M. Ciubancan^{26a}, A. Clark⁴⁹, B.L. Clark⁵⁷, P.J. Clark⁴⁶, R.N. Clarke¹⁵, W. Cleland¹²⁵, C. Clement^{146a,146b}, Y. Coadou⁸⁵, M. Cobal^{164a,164c}, A. Coccaro⁴⁹, J. Cochran⁶⁴, L. Coffey²³, J.G. Cogan¹⁴³, L. Colasurdo¹⁰⁶, B. Cole³⁵, S. Cole¹⁰⁸, A.P. Colijn¹⁰⁷, J. Collot⁵⁵, T. Colombo^{58c}, G. Compostella¹⁰¹, P. Conde Muiño^{126a,126b}, E. Coniavitis⁴⁸, S.H. Connell^{145b}, I.A. Connolly⁷⁷, V. Consorti⁴⁸, S. Constantinescu^{26a}, C. Conta^{121a,121b}, G. Conti³⁰, F. Conventi^{104a,j}, M. Cooke¹⁵, B.D. Cooper⁷⁸, A.M. Cooper-Sarkar¹²⁰, T. Cornelissen¹⁷⁵, M. Corradi^{20a}, F. Corriveau^{87,k}, A. Corso-Radu¹⁶³, A. Cortes-Gonzalez¹², G. Cortiana¹⁰¹, G. Costa^{91a}, M.J. Costa¹⁶⁷, D. Costanzo¹³⁹, D. Côté⁸, G. Cottin²⁸, G. Cowan⁷⁷, B.E. Cox⁸⁴, K. Cranmer¹¹⁰, G. Cree²⁹, S. Crépe-Renaudin⁵⁵, F. Crescioli⁸⁰, W.A. Cribbs^{146a,146b}, M. Crispin Ortuzar¹²⁰, M. Cristinziani²¹, V. Croft¹⁰⁶, G. Crosetti^{37a,37b}, T. Cuhadar Donszelmann¹³⁹, J. Cummings¹⁷⁶, M. Curatolo⁴⁷, C. Cuthbert¹⁵⁰, H. Czirr¹⁴¹, P. Czodrowski³, S. D'Auria⁵³, M. D'Onofrio⁷⁴, M.J. Da Cunha Sargedass De Sousa^{126a,126b}, C. Da Via⁸⁴, W. Dabrowski^{38a}, A. Dafinca¹²⁰, T. Dai⁸⁹, O. Dale¹⁴, F. Dallaire⁹⁵, C. Dallapiccola⁸⁶, M. Dam³⁶, J.R. Dandoy³¹, N.P. Dang⁴⁸, A.C. Daniells¹⁸, M. Danninger¹⁶⁸, M. Dano Hoffmann¹³⁶, V. Dao⁴⁸, G. Darbo^{50a}, S. Darmora⁸, J. Dassoulas³, A. Dattagupta⁶¹, W. Davey²¹, C. David¹⁶⁹, T. Davidek¹²⁹, E. Davies^{120,l}, M. Davies¹⁵³, P. Davison⁷⁸, Y. Davygora^{58a}, E. Dawe⁸⁸, I. Dawson¹³⁹, R.K. Daya-Ishmukhametova⁸⁶, K. De⁸, R. de Asmundis^{104a}, A. De Benedetti¹¹³, S. De Castro^{20a,20b}, S. De Cecco⁸⁰, N. De Groot¹⁰⁶, P. de Jong¹⁰⁷, H. De la Torre⁸², F. De Lorenzi⁶⁴, D. De Pedis^{132a}, A. De Salvo^{132a}, U. De Sanctis¹⁴⁹, A. De Santo¹⁴⁹, J.B. De Vivie De Regie¹¹⁷, W.J. Dearnaley⁷², R. Debbe²⁵, C. Debenedetti¹³⁷, D.V. Dedovich⁶⁵, I. Deigaard¹⁰⁷, J. Del Peso⁸², T. Del Prete^{124a,124b}, D. Delgove¹¹⁷, F. Deliot¹³⁶, C.M. Delitzsch⁴⁹, M. Deliyergiyev⁷⁵, A. Dell'Acqua³⁰, L. Dell'Asta²², M. Dell'Orso^{124a,124b}, M. Della Pietra^{104a,j}, D. della Volpe⁴⁹, M. Delmastro⁵, P.A. Delsart⁵⁵, C. Deluca¹⁰⁷, D.A. DeMarco¹⁵⁸, S. Demers¹⁷⁶, M. Demichev⁶⁵, A. Demilly⁸⁰, S.P. Denisov¹³⁰, D. Derendarz³⁹, J.E. Derkaoui^{135d}, F. Derue⁸⁰, P. Dervan⁷⁴, K. Desch²¹, C. Deterre⁴², P.O. Deviveiros³⁰, A. Dewhurst¹³¹, S. Dhaliwal²³, A. Di Ciaccio^{133a,133b}, L. Di Ciaccio⁵, A. Di Domenico^{132a,132b}, C. Di Donato^{104a,104b}, A. Di Girolamo³⁰, B. Di Girolamo³⁰, A. Di Mattia¹⁵², B. Di Micco^{134a,134b}, R. Di Nardo⁴⁷, A. Di Simone⁴⁸, R. Di Sipio¹⁵⁸, D. Di Valentino²⁹, C. Diaconu⁸⁵, M. Diamond¹⁵⁸, F.A. Dias⁴⁶, M.A. Diaz^{32a}, E.B. Diehl⁸⁹, J. Dietrich¹⁶, S. Diglio⁸⁵, A. Dimitrievska¹³, J. Dingfelder²¹, P. Dita^{26a}, S. Dita^{26a}, F. Dittus³⁰, F. Djama⁸⁵, T. Djobava^{51b}, J.I. Djuvsland^{58a}, M.A.B. do Vale^{24c}, D. Dobos³⁰, M. Dobre^{26a}, C. Doglioni⁸¹, T. Dohmae¹⁵⁵, J. Dolejsi¹²⁹, Z. Dolezal¹²⁹, B.A. Dolgoshein^{98,*}, M. Donadelli^{24d}, S. Donati^{124a,124b}, P. Dondero^{121a,121b}, J. Donini³⁴, J. Dopke¹³¹, A. Doria^{104a}, M.T. Dova⁷¹, A.T. Doyle⁵³, E. Drechsler⁵⁴, M. Dris¹⁰, E. Dubreuil³⁴, E. Duchovni¹⁷², G. Duckeck¹⁰⁰,

O.A. Ducu^{26a,85}, D. Duda¹⁰⁷, A. Dudarev³⁰, L. Duflost¹¹⁷, L. Duguid⁷⁷, M. Dührssen³⁰, M. Dunford^{58a}, H. Duran Yildiz^{4a}, M. Düren⁵², A. Durglishvili^{51b}, D. Duschinger⁴⁴, M. Dyndal^{38a}, C. Eckardt⁴², K.M. Ecker¹⁰¹, R.C. Edgar⁸⁹, W. Edson², N.C. Edwards⁴⁶, W. Ehrenfeld²¹, T. Eifert³⁰, G. Eigen¹⁴, K. Einsweiler¹⁵, T. Ekelof¹⁶⁶, M. El Kacimi^{135c}, M. Ellert¹⁶⁶, S. Elles⁵, F. Ellinghaus¹⁷⁵, A.A. Elliot¹⁶⁹, N. Ellis³⁰, J. Elmsheuser¹⁰⁰, M. Elsing³⁰, D. Emeliyanov¹³¹, Y. Enari¹⁵⁵, O.C. Endner⁸³, M. Endo¹¹⁸, J. Erdmann⁴³, A. Ereditato¹⁷, G. Ernis¹⁷⁵, J. Ernst², M. Ernst²⁵, S. Errede¹⁶⁵, E. Ertel⁸³, M. Escalier¹¹⁷, H. Esch⁴³, C. Escobar¹²⁵, B. Esposito⁴⁷, A.I. Etienvre¹³⁶, E. Etzion¹⁵³, H. Evans⁶¹, A. Ezhilov¹²³, L. Fabbri^{20a,20b}, G. Facini³¹, R.M. Fakhruddinov¹³⁰, S. Falciano^{132a}, R.J. Falla⁷⁸, J. Faltova¹²⁹, Y. Fang^{33a}, M. Fanti^{91a,91b}, A. Farbin⁸, A. Farilla^{134a}, T. Farooque¹², S. Farrell¹⁵, S.M. Farrington¹⁷⁰, P. Farthouat³⁰, F. Fassi^{135e}, P. Fasnacht³⁰, D. Fassouliotis⁹, M. Faucci Giannelli⁷⁷, A. Favareto^{50a,50b}, L. Fayard¹¹⁷, P. Federic^{144a}, O.L. Fedin^{123,m}, W. Fedorko¹⁶⁸, S. Feigl³⁰, L. Feligioni⁸⁵, C. Feng^{33d}, E.J. Feng⁶, H. Feng⁸⁹, A.B. Fenyuk¹³⁰, L. Feremenga⁸, P. Fernandez Martinez¹⁶⁷, S. Fernandez Perez³⁰, J. Ferrando⁵³, A. Ferrari¹⁶⁶, P. Ferrari¹⁰⁷, R. Ferrari^{121a}, D.E. Ferreira de Lima⁵³, A. Ferrer¹⁶⁷, D. Ferrere⁴⁹, C. Ferretti⁸⁹, A. Ferretto Parodi^{50a,50b}, M. Fiascaris³¹, F. Fiedler⁸³, A. Filipčič⁷⁵, M. Filipuzzi⁴², F. Filthaut¹⁰⁶, M. Fincke-Keeler¹⁶⁹, K.D. Finelli¹⁵⁰, M.C.N. Fiolhais^{126a,126c}, L. Fiorini¹⁶⁷, A. Firan⁴⁰, A. Fischer², C. Fischer¹², J. Fischer¹⁷⁵, W.C. Fisher⁹⁰, E.A. Fitzgerald²³, N. Flaschel⁴², I. Fleck¹⁴¹, P. Fleischmann⁸⁹, S. Fleischmann¹⁷⁵, G.T. Fletcher¹³⁹, G. Fletcher⁷⁶, R.R.M. Fletcher¹²², T. Flick¹⁷⁵, A. Floderus⁸¹, L.R. Flores Castillo^{60a}, M.J. Flowerdew¹⁰¹, A. Formica¹³⁶, A. Forti⁸⁴, D. Fournier¹¹⁷, H. Fox⁷², S. Fracchia¹², P. Francavilla⁸⁰, M. Franchini^{20a,20b}, D. Francis³⁰, L. Franconi¹¹⁹, M. Franklin⁵⁷, M. Frate¹⁶³, M. Fraternali^{121a,121b}, D. Freeborn⁷⁸, S.T. French²⁸, F. Friedrich⁴⁴, D. Froidevaux³⁰, J.A. Frost¹²⁰, C. Fukunaga¹⁵⁶, E. Fullana Torregrosa⁸³, B.G. Fulsom¹⁴³, T. Fusayas¹⁰², J. Fuster¹⁶⁷, C. Gabaldon⁵⁵, O. Gabizon¹⁷⁵, A. Gabrielli^{20a,20b}, A. Gabrielli^{132a,132b}, G.P. Gach^{38a}, S. Gadatsch³⁰, S. Gadomski⁴⁹, G. Gagliardi^{50a,50b}, P. Gagnon⁶¹, C. Galea¹⁰⁶, B. Galhardo^{126a,126c}, E.J. Gallas¹²⁰, B.J. Gallop¹³¹, P. Gallus¹²⁸, G. Galster³⁶, K.K. Gan¹¹¹, J. Gao^{33b,85}, Y. Gao⁴⁶, Y.S. Gao^{143,e}, F.M. Garay Walls⁴⁶, F. Garbersen¹⁷⁶, C. García¹⁶⁷, J.E. García Navarro¹⁶⁷, M. Garcia-Sciveres¹⁵, R.W. Gardner³¹, N. Garelli¹⁴³, V. Garonne¹¹⁹, C. Gatti⁴⁷, A. Gaudiello^{50a,50b}, G. Gaudio^{121a}, B. Gaur¹⁴¹, L. Gauthier⁹⁵, P. Gauzzi^{132a,132b}, I.L. Gavrilenko⁹⁶, C. Gay¹⁶⁸, G. Gaycken²¹, E.N. Gazis¹⁰, P. Ge^{33d}, Z. Gecse¹⁶⁸, C.N.P. Gee¹³¹, Ch. Geich-Gimbel²¹, M.P. Geisler^{58a}, C. Gemme^{50a}, M.H. Genest⁵⁵, S. Gentile^{132a,132b}, M. George⁵⁴, S. George⁷⁷, D. Gerbaudo¹⁶³, A. Gershon¹⁵³, S. Ghasemi¹⁴¹, H. Ghazlane^{135b}, B. Giacobbe^{20a}, S. Giagu^{132a,132b}, V. Giangiobbe¹², P. Giannetti^{124a,124b}, B. Gibbard²⁵, S.M. Gibson⁷⁷, M. Gilchriese¹⁵, T.P.S. Gillam²⁸, D. Gillberg³⁰, G. Gilles³⁴, D.M. Gingrich^{3,d}, N. Giokaris⁹, M.P. Giordani^{164a,164c}, F.M. Giorgi^{20a}, F.M. Giorgi¹⁶, P.F. Giraud¹³⁶, P. Giromini⁴⁷, D. Giugni^{91a}, C. Giuliani⁴⁸, M. Giulini^{58b}, B.K. Gjelsten¹¹⁹, S. Gkaitatzis¹⁵⁴, I. Gkialas¹⁵⁴, E.L. Gkoukousis¹¹⁷, L.K. Gladilin⁹⁹, C. Glasman⁸², J. Glatzer³⁰, P.C.F. Glaysheer⁴⁶, A. Glazov⁴², M. Goblirsch-Kolb¹⁰¹, J.R. Goddard⁷⁶, J. Godlewski³⁹, S. Goldfarb⁸⁹, T. Golling⁴⁹, D. Golubkov¹³⁰, A. Gomes^{126a,126b,126d}, R. Gonçalo^{126a}, J. Goncalves Pinto Firmino Da Costa¹³⁶, L. Gonella²¹, S. González de la Hoz¹⁶⁷, G. Gonzalez Parra¹², S. Gonzalez-Sevilla⁴⁹, L. Goossens³⁰, P.A. Gorbounov⁹⁷, H.A. Gordon²⁵, I. Gorelov¹⁰⁵, B. Gorini³⁰, E. Gorini^{73a,73b}, A. Gorišek⁷⁵, E. Gornicki³⁹, A.T. Goshaw⁴⁵, C. Gössling⁴³, M.I. Gostkin⁶⁵, D. Goujdami^{135c}, A.G. Goussiou¹³⁸, N. Govender^{145b}, E. Gozani¹⁵², H.M.X. Grabas¹³⁷, L. Graber⁵⁴, I. Grabowska-Bold^{38a}, P.O.J. Gradin¹⁶⁶, P. Grafström^{20a,20b}, K.-J. Grah⁴², J. Gramling⁴⁹, E. Gramstad¹¹⁹, S. Grancagnolo¹⁶, V. Gratchev¹²³, H.M. Gray³⁰, E. Graziani^{134a}, Z.D. Greenwood^{79,n}, C. Grefe²¹, K. Gregersen⁷⁸, I.M. Gregor⁴², P. Grenier¹⁴³, J. Griffiths⁸, A.A. Grillo¹³⁷, K. Grimm⁷², S. Grinstein^{12,o}, Ph. Gris³⁴, J.-F. Grivaz¹¹⁷, J.P. Grohs⁴⁴, A. Grohsjean⁴², E. Gross¹⁷², J. Grosse-Knetter⁵⁴, G.C. Grossi⁷⁹, Z.J. Grout¹⁴⁹, L. Guan⁸⁹, J. Guenther¹²⁸, F. Guescini⁴⁹, D. Guest¹⁷⁶, O. Gueta¹⁵³, E. Guido^{50a,50b}, T. Guillemin¹¹⁷, S. Guindon², U. Gul⁵³, C. Gumpert⁴⁴, J. Guo^{33e}, Y. Guo^{33b}, S. Gupta¹²⁰, G. Gustavino^{132a,132b}, P. Gutierrez¹¹³, N.G. Gutierrez Ortiz⁷⁸, C. Gutsche⁴⁴, C. Guyot¹³⁶, C. Gwenlan¹²⁰, C.B. Gwilliam⁷⁴, A. Haas¹¹⁰, C. Haber¹⁵, H.K. Hadavand⁸, N. Haddad^{135e}, P. Haefner²¹, S. Hageböck²¹, Z. Hajduk³⁹, H. Hakobyan¹⁷⁷, M. Haleem⁴², J. Haley¹¹⁴, D. Hall¹²⁰, G. Halladjian⁹⁰, G.D. Hallowell⁸⁵, K. Hamacher¹⁷⁵, P. Hamal¹¹⁵, K. Hamano¹⁶⁹, A. Hamilton^{145a}, G.N. Hamity¹³⁹, P.G. Hamnett⁴², L. Han^{33b}, K. Hanagaki^{66,p}, K. Hanawa¹⁵⁵, M. Hance¹⁵, P. Hanke^{58a}, R. Hanna¹³⁶, J.B. Hansen³⁶, J.D. Hansen³⁶, M.C. Hansen²¹, P.H. Hansen³⁶, K. Hara¹⁶⁰, A.S. Hard¹⁷³, T. Harenberg¹⁷⁵, F. Hariri¹¹⁷, S. Harkusha⁹², R.D. Harrington⁴⁶, P.F. Harrison¹⁷⁰, F. Hartjes¹⁰⁷, M. Hasegawa⁶⁷,

Y. Hasegawa¹⁴⁰, A. Hasib¹¹³, S. Hassani¹³⁶, S. Haug¹⁷, R. Hauser⁹⁰, L. Hauswald⁴⁴, M. Havranek¹²⁷, C.M. Hawkes¹⁸, R.J. Hawking³⁰, A.D. Hawkins⁸¹, T. Hayashi¹⁶⁰, D. Hayden⁹⁰, C.P. Hays¹²⁰, J.M. Hays⁷⁶, H.S. Hayward⁷⁴, S.J. Haywood¹³¹, S.J. Head¹⁸, T. Heck⁸³, V. Hedberg⁸¹, L. Heelan⁸, S. Heim¹²², T. Heim¹⁷⁵, B. Heinemann¹⁵, L. Heinrich¹¹⁰, J. Hejbal¹²⁷, L. Helary²², S. Hellman^{146a,146b}, D. Hellmich²¹, C. Helsens¹², J. Henderson¹²⁰, R.C.W. Henderson⁷², Y. Heng¹⁷³, C. Hengler⁴², S. Henkelmann¹⁶⁸, A. Henrichs¹⁷⁶, A.M. Henriques Correia³⁰, S. Henrot-Versille¹¹⁷, G.H. Herbert¹⁶, Y. Hernández Jiménez¹⁶⁷, R. Herrberg-Schubert¹⁶, G. Herten⁴⁸, R. Hertenberger¹⁰⁰, L. Hervas³⁰, G.G. Hesketh⁷⁸, N.P. Hessey¹⁰⁷, J.W. Hetherly⁴⁰, R. Hickling⁷⁶, E. Higón-Rodríguez¹⁶⁷, E. Hill¹⁶⁹, J.C. Hill²⁸, K.H. Hiller⁴², S.J. Hillier¹⁸, I. Hinchliffe¹⁵, E. Hines¹²², R.R. Hinman¹⁵, M. Hirose¹⁵⁷, D. Hirschbuehl¹⁷⁵, J. Hobbs¹⁴⁸, N. Hod¹⁰⁷, M.C. Hodgkinson¹³⁹, P. Hodgson¹³⁹, A. Hoecker³⁰, M.R. Hoferkamp¹⁰⁵, F. Hoenig¹⁰⁰, M. Hohlfield⁸³, D. Hohn²¹, T.R. Holmes¹⁵, M. Homann⁴³, T.M. Hong¹²⁵, L. Hooft van Huysduynen¹¹⁰, W.H. Hopkins¹¹⁶, Y. Horii¹⁰³, A.J. Horton¹⁴², J.-Y. Hostachy⁵⁵, S. Hou¹⁵¹, A. Hoummada^{135a}, J. Howard¹²⁰, J. Howarth⁴², M. Hrabovsky¹¹⁵, I. Hristova¹⁶, J. Hrivnac¹¹⁷, T. Hryn'ova⁵, A. Hrynevich⁹³, C. Hsu^{145c}, P.J. Hsu^{151,q}, S.-C. Hsu¹³⁸, D. Hu³⁵, Q. Hu^{33b}, X. Hu⁸⁹, Y. Huang⁴², Z. Hubacek¹²⁸, F. Hubaut⁸⁵, F. Huegging²¹, T.B. Huffman¹²⁰, E.W. Hughes³⁵, G. Hughes⁷², M. Huhtinen³⁰, T.A. Hülsing⁸³, N. Huseynov^{65,b}, J. Huston⁹⁰, J. Huth⁵⁷, G. Iacobucci⁴⁹, G. Iakovidis²⁵, I. Ibragimov¹⁴¹, L. Iconomidou-Fayard¹¹⁷, E. Ideal¹⁷⁶, Z. Idrissi^{135e}, P. Iengo³⁰, O. Igonkina¹⁰⁷, T. Iizawa¹⁷¹, Y. Ikegami⁶⁶, K. Ikematsu¹⁴¹, M. Ikeno⁶⁶, Y. Ilchenko^{31,r}, D. Iliadis¹⁵⁴, N. Ilic¹⁴³, T. Ince¹⁰¹, G. Introzzi^{121a,121b}, P. Ioannou⁹, M. Iodice^{134a}, K. Iordanidou³⁵, V. Ippolito⁵⁷, A. Irles Quiles¹⁶⁷, C. Isaksson¹⁶⁶, M. Ishino⁶⁸, M. Ishitsuka¹⁵⁷, R. Ishmukhametov¹¹¹, C. Issever¹²⁰, S. Istin^{19a}, J.M. Iturbe Ponce⁸⁴, R. Iuppa^{133a,133b}, J. Ivarsson⁸¹, W. Iwanski³⁹, H. Iwasaki⁶⁶, J.M. Izen⁴¹, V. Izzo^{104a}, S. Jabbar³, B. Jackson¹²², M. Jackson⁷⁴, P. Jackson¹, M.R. Jaekel³⁰, V. Jain², K. Jakobs⁴⁸, S. Jakobsen³⁰, T. Jakoubek¹²⁷, J. Jakubek¹²⁸, D.O. Jamin¹¹⁴, D.K. Jana⁷⁹, E. Jansen⁷⁸, R. Jansky⁶², J. Janssen²¹, M. Janus⁵⁴, G. Jarlskog⁸¹, N. Javadov^{65,b}, T. Javůrek⁴⁸, L. Jeanty¹⁵, J. Jejelava^{51a,s}, G.-Y. Jeng¹⁵⁰, D. Jennens⁸⁸, P. Jenni^{48,t}, J. Jentzsch⁴³, C. Jeske¹⁷⁰, S. Jézéquel⁵, H. Ji¹⁷³, J. Jia¹⁴⁸, Y. Jiang^{33b}, S. Jiggins⁷⁸, J. Jimenez Pena¹⁶⁷, S. Jin^{33a}, A. Jinaru^{26a}, O. Jinnouchi¹⁵⁷, M.D. Joergensen³⁶, P. Johansson¹³⁹, K.A. Johns⁷, K. Jon-And^{146a,146b}, G. Jones¹⁷⁰, R.W.L. Jones⁷², T.J. Jones⁷⁴, J. Jongmanns^{58a}, P.M. Jorge^{126a,126b}, K.D. Joshi⁸⁴, J. Jovicevic^{159a}, X. Ju¹⁷³, C.A. Jung⁴³, P. Jussel⁶², A. Juste Rozas^{12,o}, M. Kaci¹⁶⁷, A. Kaczmarska³⁹, M. Kado¹¹⁷, H. Kagan¹¹¹, M. Kagan¹⁴³, S.J. Kahn⁸⁵, E. Kajomovitz⁴⁵, C.W. Kalderon¹²⁰, S. Kama⁴⁰, A. Kamenshchikov¹³⁰, N. Kanaya¹⁵⁵, S. Kaneti²⁸, V.A. Kantserov⁹⁸, J. Kanzaki⁶⁶, B. Kaplan¹¹⁰, L.S. Kaplan¹⁷³, A. Kapliy³¹, D. Kar^{145c}, K. Karakostas¹⁰, A. Karamaoun³, N. Karastathis^{10,107}, M.J. Kareem⁵⁴, E. Karentzos¹⁰, M. Karnevskiy⁸³, S.N. Karpov⁶⁵, Z.M. Karpova⁶⁵, K. Karthik¹¹⁰, V. Kartvelishvili⁷², A.N. Karyukhin¹³⁰, L. Kashif¹⁷³, R.D. Kass¹¹¹, A. Kastanas¹⁴, Y. Kataoka¹⁵⁵, C. Kato¹⁵⁵, A. Katre⁴⁹, J. Katzy⁴², K. Kawagoe⁷⁰, T. Kawamoto¹⁵⁵, G. Kawamura⁵⁴, S. Kazama¹⁵⁵, V.F. Kazanin^{109,c}, R. Keeler¹⁶⁹, R. Kehoe⁴⁰, J.S. Keller⁴², J.J. Kempster⁷⁷, H. Keoshkerian⁸⁴, O. Kepka¹²⁷, B.P. Kerševan⁷⁵, S. Kersten¹⁷⁵, R.A. Keyes⁸⁷, F. Khalil-zada¹¹, H. Khandanyan^{146a,146b}, A. Khanov¹¹⁴, A.G. Kharlamov^{109,c}, T.J. Khoo²⁸, V. Khovanskiy⁹⁷, E. Khramov⁶⁵, J. Khubua^{51b,u}, S. Kido⁶⁷, H.Y. Kim⁸, S.H. Kim¹⁶⁰, Y.K. Kim³¹, N. Kimura¹⁵⁴, O.M. Kind¹⁶, B.T. King⁷⁴, M. King¹⁶⁷, S.B. King¹⁶⁸, J. Kirk¹³¹, A.E. Kiryunin¹⁰¹, T. Kishimoto⁶⁷, D. Kisielewska^{38a}, F. Kiss⁴⁸, K. Kiuchi¹⁶⁰, O. Kivernyk¹³⁶, E. Kladiva^{144b}, M.H. Klein³⁵, M. Klein⁷⁴, U. Klein⁷⁴, K. Kleinknecht⁸³, P. Klimek^{146a,146b}, A. Klimentov²⁵, R. Klingenberg⁴³, J.A. Klinger¹³⁹, T. Klioutchnikova³⁰, E.-E. Kluge^{58a}, P. Kluit¹⁰⁷, S. Kluth¹⁰¹, J. Knapik³⁹, E. Kneringer⁶², E.B.F.G. Knoop⁸⁵, A. Knue⁵³, A. Kobayashi¹⁵⁵, D. Kobayashi¹⁵⁷, T. Kobayashi¹⁵⁵, M. Kobel⁴⁴, M. Kocian¹⁴³, P. Kodys¹²⁹, T. Koffas²⁹, E. Koffeman¹⁰⁷, L.A. Kogan¹²⁰, S. Kohlmann¹⁷⁵, Z. Kohout¹²⁸, T. Kohriki⁶⁶, T. Koi¹⁴³, H. Kolanoski¹⁶, I. Koletsou⁵, A.A. Komar^{96,*}, Y. Komori¹⁵⁵, T. Kondo⁶⁶, N. Kondrashova⁴², K. Köneke⁴⁸, A.C. König¹⁰⁶, T. Kono⁶⁶, R. Konoplich^{110,v}, N. Konstantinidis⁷⁸, R. Kopeliansky¹⁵², S. Koperny^{38a}, L. Köpke⁸³, A.K. Kopp⁴⁸, K. Korcyl³⁹, K. Kordas¹⁵⁴, A. Korn⁷⁸, A.A. Korol^{109,c}, I. Korolkov¹², E.V. Korolkova¹³⁹, O. Kortner¹⁰¹, S. Kortner¹⁰¹, T. Kosek¹²⁹, V.V. Kostyukhin²¹, V.M. Kotov⁶⁵, A. Kotwal⁴⁵, A. Kourkoumeli-Charalampidi¹⁵⁴, C. Kourkoumelis⁹, V. Kouskoura²⁵, A. Koutsman^{159a}, R. Kowalewski¹⁶⁹, T.Z. Kowalski^{38a}, W. Kozanecki¹³⁶, A.S. Kozhin¹³⁰, V.A. Kramarenko⁹⁹, G. Kramberger⁷⁵, D. Krasnopevtsev⁹⁸, M.W. Krasny⁸⁰, A. Krasznahorkay³⁰, J.K. Kraus²¹, A. Kravchenko²⁵, S. Kreiss¹¹⁰, M. Kretz^{58c}, J. Kretzschmar⁷⁴, K. Kreutzfeldt⁵², P. Krieger¹⁵⁸,

K. Krizka³¹, K. Kroeninger⁴³, H. Kroha¹⁰¹, J. Kroll¹²², J. Kroseberg²¹, J. Krstic¹³, U. Kruchonak⁶⁵, H. Krüger²¹, N. Krumnack⁶⁴, A. Kruse¹⁷³, M.C. Kruse⁴⁵, M. Kruskal²², T. Kubota⁸⁸, H. Kucuk⁷⁸, S. Kuday^{4b}, S. Kuehn⁴⁸, A. Kugel^{58c}, F. Kuger¹⁷⁴, A. Kuhl¹³⁷, T. Kuhl⁴², V. Kukhtin⁶⁵, R. Kukla¹³⁶, Y. Kulchitsky⁹², S. Kuleshov^{32b}, M. Kuna^{132a,132b}, T. Kunigo⁶⁸, A. Kupco¹²⁷, H. Kurashige⁶⁷, Y.A. Kurochkin⁹², V. Kus¹²⁷, E.S. Kuwertz¹⁶⁹, M. Kuze¹⁵⁷, J. Kvita¹¹⁵, T. Kwan¹⁶⁹, D. Kyriazopoulos¹³⁹, A. La Rosa¹³⁷, J.L. La Rosa Navarro^{24d}, L. La Rotonda^{37a,37b}, C. Lacasta¹⁶⁷, F. Lacava^{132a,132b}, J. Lacey²⁹, H. Lacker¹⁶, D. Lacour⁸⁰, V.R. Lacuesta¹⁶⁷, E. Ladygin⁶⁵, R. Lafaye⁵, B. Laforge⁸⁰, T. Lagouri¹⁷⁶, S. Lai⁵⁴, L. Lambourne⁷⁸, S. Lammers⁶¹, C.L. Lampen⁷, W. Lampl⁷, E. Lançon¹³⁶, U. Landgraf⁴⁸, M.P.J. Landon⁷⁶, V.S. Lang^{58a}, J.C. Lange¹², A.J. Lankford¹⁶³, F. Lanni²⁵, K. Lantzscht²¹, A. Lanza^{121a}, S. Laplace⁸⁰, C. Lapoire³⁰, J.F. Laporte¹³⁶, T. Lari^{91a}, F. Lasagni Manghi^{20a,20b}, M. Lassnig³⁰, P. Laurelli⁴⁷, W. Lavrijsen¹⁵, A.T. Law¹³⁷, P. Laycock⁷⁴, T. Lazovich⁵⁷, O. Le Dortz⁸⁰, E. Le Guirriec⁸⁵, E. Le Menedeu¹², M. LeBlanc¹⁶⁹, T. LeCompte⁶, F. Ledroit-Guillon⁵⁵, C.A. Lee^{145b}, S.C. Lee¹⁵¹, L. Lee¹, G. Lefebvre⁸⁰, M. Lefebvre¹⁶⁹, F. Legger¹⁰⁰, C. Leggett¹⁵, A. Lehan⁷⁴, G. Lehmann Miotto³⁰, X. Lei⁷, W.A. Leight²⁹, A. Leisos^{154,w}, A.G. Leister¹⁷⁶, M.A.L. Leite^{24d}, R. Leitner¹²⁹, D. Lellouch¹⁷², B. Lemmer⁵⁴, K.J.C. Leney⁷⁸, T. Lenz²¹, B. Lenzi³⁰, R. Leone⁷, S. Leone^{124a,124b}, C. Leonidopoulos⁴⁶, S. Leontsinis¹⁰, C. Leroy⁹⁵, C.G. Lester²⁸, M. Levchenko¹²³, J. Levêque⁵, D. Levin⁸⁹, L.J. Levinson¹⁷², M. Levy¹⁸, A. Lewis¹²⁰, A.M. Leyko²¹, M. Leyton⁴¹, B. Li^{33b,x}, H. Li¹⁴⁸, H.L. Li³¹, L. Li⁴⁵, L. Li^{33e}, S. Li⁴⁵, X. Li⁸⁴, Y. Li^{33c,y}, Z. Liang¹³⁷, H. Liao³⁴, B. Liberti^{133a}, A. Liblong¹⁵⁸, P. Lichard³⁰, K. Lie¹⁶⁵, J. Liebal²¹, W. Liebig¹⁴, C. Limbach²¹, A. Limosani¹⁵⁰, S.C. Lin^{151,z}, T.H. Lin⁸³, F. Linde¹⁰⁷, B.E. Lindquist¹⁴⁸, J.T. Linnemann⁹⁰, E. Lipeles¹²², A. Lipniacka¹⁴, M. Lisovyi^{58b}, T.M. Liss¹⁶⁵, D. Lissauer²⁵, A. Lister¹⁶⁸, A.M. Litke¹³⁷, B. Liu^{151,aa}, D. Liu¹⁵¹, H. Liu⁸⁹, J. Liu⁸⁵, J.B. Liu^{33b}, K. Liu⁸⁵, L. Liu¹⁶⁵, M. Liu⁴⁵, M. Liu^{33b}, Y. Liu^{33b}, M. Livan^{121a,121b}, A. Lleres⁵⁵, J. Llorente Merino⁸², S.L. Lloyd⁷⁶, F. Lo Sterzo¹⁵¹, E. Lobodzinska⁴², P. Loch⁷, W.S. Lockman¹³⁷, F.K. Loebinger⁸⁴, A.E. Loevschall-Jensen³⁶, A. Loginov¹⁷⁶, T. Lohse¹⁶, K. Lohwasser⁴², M. Lokajicek¹²⁷, B.A. Long²², J.D. Long⁸⁹, R.E. Long⁷², K.A. Looper¹¹¹, L. Lopes^{126a}, D. Lopez Mateos⁵⁷, B. Lopez Paredes¹³⁹, I. Lopez Paz¹², J. Lorenz¹⁰⁰, N. Lorenzo Martinez⁶¹, M. Losada¹⁶², P.J. Lösel¹⁰⁰, X. Lou^{33a}, A. Lounis¹¹⁷, J. Love⁶, P.A. Love⁷², N. Lu⁸⁹, H.J. Lubatti¹³⁸, C. Luci^{132a,132b}, A. Lucotte⁵⁵, F. Luehring⁶¹, W. Lukas⁶², L. Luminari^{132a}, O. Lundberg^{146a,146b}, B. Lund-Jensen¹⁴⁷, D. Lynn²⁵, R. Lysak¹²⁷, E. Lytken⁸¹, H. Ma²⁵, L.L. Ma^{33d}, G. Maccarrone⁴⁷, A. Macchiolo¹⁰¹, C.M. Macdonald¹³⁹, B. Maček⁷⁵, J. Machado Miguens^{122,126b}, D. Macina³⁰, D. Madaffari⁸⁵, R. Madar³⁴, H.J. Maddocks⁷², W.F. Mader⁴⁴, A. Madsen¹⁶⁶, J. Maeda⁶⁷, S. Maeland¹⁴, T. Maeno²⁵, A. Maevskiy⁹⁹, E. Magradze⁵⁴, K. Mahboubi⁴⁸, J. Mahlstedt¹⁰⁷, C. Maiani¹³⁶, C. Maidantchik^{24a}, A.A. Maier¹⁰¹, T. Maier¹⁰⁰, A. Maio^{126a,126b,126d}, S. Majewski¹¹⁶, Y. Makida⁶⁶, N. Makovec¹¹⁷, B. Malaescu⁸⁰, Pa. Malecki³⁹, V.P. Maleev¹²³, F. Malek⁵⁵, U. Mallik⁶³, D. Malon⁶, C. Malone¹⁴³, S. Maltezos¹⁰, V.M. Malyshev¹⁰⁹, S. Malyukov³⁰, J. Mamuzic⁴², G. Mancini⁴⁷, B. Mandelli³⁰, L. Mandelli^{91a}, I. Mandić⁷⁵, R. Mandrysch⁶³, J. Maneira^{126a,126b}, A. Manfredini¹⁰¹, L. Manhaes de Andrade Filho^{24b}, J. Manjarres Ramos^{159b}, A. Mann¹⁰⁰, A. Manousakis-Katsikakis⁹, B. Mansoulie¹³⁶, R. Mantifel⁸⁷, M. Mantoani⁵⁴, L. Mapelli³⁰, L. March^{145c}, G. Marchiori⁸⁰, M. Marcisovsky¹²⁷, C.P. Marino¹⁶⁹, M. Marjanovic¹³, D.E. Marley⁸⁹, F. Marroquim^{24a}, S.P. Marsden⁸⁴, Z. Marshall¹⁵, L.F. Marti¹⁷, S. Marti-Garcia¹⁶⁷, B. Martin⁹⁰, T.A. Martin¹⁷⁰, V.J. Martin⁴⁶, B. Martin dit Latour¹⁴, M. Martinez^{12,o}, S. Martin-Haugh¹³¹, V.S. Martoiu^{26a}, A.C. Martyniuk⁷⁸, M. Marx¹³⁸, F. Marzano^{132a}, A. Marzin³⁰, L. Masetti⁸³, T. Mashimo¹⁵⁵, R. Mashinistov⁹⁶, J. Masik⁸⁴, A.L. Maslennikov^{109,c}, I. Massa^{20a,20b}, L. Massa^{20a,20b}, P. Mastrandrea¹⁴⁸, A. Mastroberardino^{37a,37b}, T. Masubuchi¹⁵⁵, P. Mättig¹⁷⁵, J. Mattmann⁸³, J. Maurer^{26a}, S.J. Maxfield⁷⁴, D.A. Maximov^{109,c}, R. Mazini¹⁵¹, S.M. Mazza^{91a,91b}, L. Mazzaferro^{133a,133b}, G. Mc Goldrick¹⁵⁸, S.P. Mc Kee⁸⁹, A. McCarn⁸⁹, R.L. McCarthy¹⁴⁸, T.G. McCarthy²⁹, N.A. McCubbin¹³¹, K.W. McFarlane^{56,*}, J.A. Mcfayden⁷⁸, G. Mchedlidze⁵⁴, S.J. McMahon¹³¹, R.A. McPherson^{169,k}, M. Medinnis⁴², S. Meehan^{145a}, S. Mehlhase¹⁰⁰, A. Mehta⁷⁴, K. Meier^{58a}, C. Meineck¹⁰⁰, B. Meirose⁴¹, B.R. Mellado Garcia^{145c}, F. Meloni¹⁷, A. Mengarelli^{20a,20b}, S. Menke¹⁰¹, E. Meoni¹⁶¹, K.M. Mercurio⁵⁷, S. Mergelmeyer²¹, P. Mermod⁴⁹, L. Merola^{104a,104b}, C. Meroni^{91a}, F.S. Merritt³¹, A. Messina^{132a,132b}, J. Metcalfe²⁵, A.S. Mete¹⁶³, C. Meyer⁸³, C. Meyer¹²², J.-P. Meyer¹³⁶, J. Meyer¹⁰⁷, H. Meyer Zu Theenhausen^{58a}, R.P. Middleton¹³¹, S. Miglioranza^{164a,164c}, L. Mijović²¹, G. Mikenberg¹⁷², M. Mikestikova¹²⁷, M. Mikuž⁷⁵, M. Milesi⁸⁸, A. Milic³⁰, D.W. Miller³¹, C. Mills⁴⁶, A. Milov¹⁷², D.A. Milstead^{146a,146b}, A.A. Minaenko¹³⁰,

Y. Minami¹⁵⁵, I.A. Minashvili⁶⁵, A.I. Mincer¹¹⁰, B. Mindur^{38a}, M. Mineev⁶⁵, Y. Ming¹⁷³, L.M. Mir¹², T. Mitani¹⁷¹, J. Mitrevski¹⁰⁰, V.A. Mitsou¹⁶⁷, A. Miucci⁴⁹, P.S. Miyagawa¹³⁹, J.U. Mjörnmark⁸¹, T. Moa^{146a,146b}, K. Mochizuki⁸⁵, S. Mohapatra³⁵, W. Mohr⁴⁸, S. Molander^{146a,146b}, R. Moles-Valls²¹, R. Monden⁶⁸, K. Mönig⁴², C. Monini⁵⁵, J. Monk³⁶, E. Monnier⁸⁵, J. Montejo Berlingen¹², F. Monticelli⁷¹, S. Monzani^{132a,132b}, R.W. Moore³, N. Morange¹¹⁷, D. Moreno¹⁶², M. Moreno Llácer⁵⁴, P. Morettini^{50a}, D. Mori¹⁴², M. Morii⁵⁷, M. Morinaga¹⁵⁵, V. Morisbak¹¹⁹, S. Moritz⁸³, A.K. Morley¹⁵⁰, G. Mornacchi³⁰, J.D. Morris⁷⁶, S.S. Mortensen³⁶, A. Morton⁵³, L. Morvaj¹⁰³, M. Mosidze^{51b}, J. Moss¹⁴³, K. Motohashi¹⁵⁷, R. Mount¹⁴³, E. Mountricha²⁵, S.V. Mouraviev^{96,*}, E.J.W. Moyse⁸⁶, S. Muanza⁸⁵, R.D. Mudd¹⁸, F. Mueller¹⁰¹, J. Mueller¹²⁵, R.S.P. Mueller¹⁰⁰, T. Mueller²⁸, D. Muenstermann⁴⁹, P. Mullen⁵³, G.A. Mullier¹⁷, J.A. Murillo Quijada¹⁸, W.J. Murray^{170,131}, H. Musheghyan⁵⁴, E. Musto¹⁵², A.G. Myagkov^{130,ab}, M. Myska¹²⁸, B.P. Nachman¹⁴³, O. Nackenhorst⁵⁴, J. Nadal⁵⁴, K. Nagai¹²⁰, R. Nagai¹⁵⁷, Y. Nagai⁸⁵, K. Nagano⁶⁶, A. Nagarkar¹¹¹, Y. Nagasaka⁵⁹, K. Nagata¹⁶⁰, M. Nagel¹⁰¹, E. Nagy⁸⁵, A.M. Nairz³⁰, Y. Nakahama³⁰, K. Nakamura⁶⁶, T. Nakamura¹⁵⁵, I. Nakano¹¹², H. Namasivayam⁴¹, R.F. Naranjo Garcia⁴², R. Narayan³¹, D.I. Narrias Villar^{58a}, T. Naumann⁴², G. Navarro¹⁶², R. Nayyar⁷, H.A. Neal⁸⁹, P.Yu. Nechaeva⁹⁶, T.J. Neep⁸⁴, P.D. Nef¹⁴³, A. Negri^{121a,121b}, M. Negrini^{20a}, S. Nektarijevic¹⁰⁶, C. Nellist¹¹⁷, A. Nelson¹⁶³, S. Nemecek¹²⁷, P. Nemethy¹¹⁰, A.A. Nepomuceno^{24a}, M. Nessi^{30,ac}, M.S. Neubauer¹⁶⁵, M. Neumann¹⁷⁵, R.M. Neves¹¹⁰, P. Nevski²⁵, P.R. Newman¹⁸, D.H. Nguyen⁶, R.B. Nickerson¹²⁰, R. Nicolaïdou¹³⁶, B. Nicquevert³⁰, J. Nielsen¹³⁷, N. Nikiforou³⁵, A. Nikiforov¹⁶, V. Nikolaenko^{130,ab}, I. Nikolic-Audit⁸⁰, K. Nikolopoulos¹⁸, J.K. Nilsen¹¹⁹, P. Nilsson²⁵, Y. Ninomiya¹⁵⁵, A. Nisati^{132a}, R. Nisius¹⁰¹, T. Nobe¹⁵⁵, M. Nomachi¹¹⁸, I. Nomidis²⁹, T. Nooney⁷⁶, S. Norberg¹¹³, M. Nordberg³⁰, O. Novgorodova⁴⁴, S. Nowak¹⁰¹, M. Nozaki⁶⁶, L. Nozka¹¹⁵, K. Ntekas¹⁰, G. Nunes Hanninger⁸⁸, T. Nunnemann¹⁰⁰, E. Nurse⁷⁸, F. Nuti⁸⁸, B.J. O'Brien⁴⁶, F. O'grady⁷, D.C. O'Neil¹⁴², V. O'Shea⁵³, F.G. Oakham^{29,d}, H. Oberlack¹⁰¹, T. Obermann²¹, J. Ocariz⁸⁰, A. Ochi⁶⁷, I. Ochoa⁷⁸, J.P. Ochoa-Ricoux^{32a}, S. Oda⁷⁰, S. Odaka⁶⁶, H. Ogren⁶¹, A. Oh⁸⁴, S.H. Oh⁴⁵, C.C. Ohm¹⁵, H. Ohman¹⁶⁶, H. Oide³⁰, W. Okamura¹¹⁸, H. Okawa¹⁶⁰, Y. Okumura³¹, T. Okuyama⁶⁶, A. Olariu^{26a}, S.A. Olivares Pino⁴⁶, D. Oliveira Damazio²⁵, E. Oliver Garcia¹⁶⁷, A. Olszewski³⁹, J. Olszowska³⁹, A. Onofre^{126a,126e}, K. Onogi¹⁰³, P.U.E. Onyisi^{31,r}, C.J. Oram^{159a}, M.J. Oreglia³¹, Y. Oren¹⁵³, D. Orestano^{134a,134b}, N. Orlando¹⁵⁴, C. Oropeza Barrera⁵³, R.S. Orr¹⁵⁸, B. Osculati^{50a,50b}, R. Ospanov⁸⁴, G. Otero y Garzon²⁷, H. Otono⁷⁰, M. Ouchrif^{135d}, F. Ould-Saada¹¹⁹, A. Ouraou¹³⁶, K.P. Oussoren¹⁰⁷, Q. Ouyang^{33a}, A. Ovcharova¹⁵, M. Owen⁵³, R.E. Owen¹⁸, V.E. Ozcan^{19a}, N. Ozturk⁸, K. Pachal¹⁴², A. Pacheco Pages¹², C. Padilla Aranda¹², M. Pagáčová⁴⁸, S. Pagan Griso¹⁵, E. Paganis¹³⁹, F. Paige²⁵, P. Pais⁸⁶, K. Pajchel¹¹⁹, G. Palacino^{159b}, S. Palestini³⁰, M. Palka^{38b}, D. Pallin³⁴, A. Palma^{126a,126b}, Y.B. Pan¹⁷³, E. Panagiotopoulou¹⁰, C.E. Pandini⁸⁰, J.G. Panduro Vazquez⁷⁷, P. Pani^{146a,146b}, S. Panitkin²⁵, D. Pantea^{26a}, L. Paolozzi⁴⁹, Th.D. Papadopoulou¹⁰, K. Papageorgiou¹⁵⁴, A. Paramonov⁶, D. Paredes Hernandez¹⁵⁴, M.A. Parker²⁸, K.A. Parker¹³⁹, F. Parodi^{50a,50b}, J.A. Parsons³⁵, U. Parzefall⁴⁸, E. Pasqualucci^{132a}, S. Passaggio^{50a}, F. Pastore^{134a,134b,*}, Fr. Pastore⁷⁷, G. Pásztor²⁹, S. Patariaia¹⁷⁵, N.D. Patel¹⁵⁰, J.R. Pater⁸⁴, T. Pauly³⁰, J. Pearce¹⁶⁹, B. Pearson¹¹³, L.E. Pedersen³⁶, M. Pedersen¹¹⁹, S. Pedraza Lopez¹⁶⁷, R. Pedro^{126a,126b}, S.V. Peleganchuk^{109,c}, D. Pelikan¹⁶⁶, O. Penc¹²⁷, C. Peng^{33a}, H. Peng^{33b}, B. Penning³¹, J. Penwell⁶¹, D.V. Perepelitsa²⁵, E. Perez Codina^{159a}, M.T. Pérez García-Estañ¹⁶⁷, L. Perini^{91a,91b}, H. Pernegger³⁰, S. Perrella^{104a,104b}, R. Peschke⁴², V.D. Peshekhonov⁶⁵, K. Peters³⁰, R.F.Y. Peters⁸⁴, B.A. Petersen³⁰, T.C. Petersen³⁶, E. Petit⁴², A. Petridis¹, C. Petridou¹⁵⁴, P. Petroff¹¹⁷, E. Petrolo^{132a}, F. Petrucci^{134a,134b}, N.E. Pettersson¹⁵⁷, R. Pezoa^{32b}, P.W. Phillips¹³¹, G. Piacquadio¹⁴³, E. Pianori¹⁷⁰, A. Picazio⁴⁹, E. Piccaro⁷⁶, M. Piccinini^{20a,20b}, M.A. Pickering¹²⁰, R. Piegai²⁷, D.T. Pignotti¹¹¹, J.E. Pilcher³¹, A.D. Pilkington⁸⁴, J. Pina^{126a,126b,126d}, M. Pinamonti^{164a,164c,ad}, J.L. Pinfold³, A. Pingel³⁶, S. Pires⁸⁰, H. Pirumov⁴², M. Pitt¹⁷², C. Pizio^{91a,91b}, L. Plazak^{144a}, M.-A. Pleier²⁵, V. Pleskot¹²⁹, E. Plotnikova⁶⁵, P. Plucinski^{146a,146b}, D. Pluth⁶⁴, R. Poettgen^{146a,146b}, L. Poggioli¹¹⁷, D. Pohl²¹, G. Polesello^{121a}, A. Poley⁴², A. Policicchio^{37a,37b}, R. Polifka¹⁵⁸, A. Polini^{20a}, C.S. Pollard⁵³, V. Polychronakos²⁵, K. Pommès³⁰, L. Pontecorvo^{132a}, B.G. Pope⁹⁰, G.A. Popeneciu^{26b}, D.S. Popovic¹³, A. Poppleton³⁰, S. Pospisil¹²⁸, K. Potamianos¹⁵, I.N. Potrap⁶⁵, C.J. Potter¹⁴⁹, C.T. Potter¹¹⁶, G. Poulard³⁰, J. Poveda³⁰, V. Pozdnyakov⁶⁵, P. Pralavorio⁸⁵, A. Pranko¹⁵, S. Prasad³⁰, S. Prell⁶⁴, D. Price⁸⁴, L.E. Price⁶, M. Primavera^{73a}, S. Prince⁸⁷, M. Proissl⁴⁶, K. Prokofiev^{60c}, F. Prokoshin^{32b}, E. Protopapadaki¹³⁶, S. Protopopescu²⁵, J. Proudfoot⁶,

M. Przybycien^{38a}, E. Ptacek¹¹⁶, D. Puddu^{134a,134b}, E. Pueschel⁸⁶, D. Poldon¹⁴⁸, M. Purohit^{25,ae},
P. Puzo¹¹⁷, J. Qian⁸⁹, G. Qin⁵³, Y. Qin⁸⁴, A. Quadt⁵⁴, D.R. Quarrie¹⁵, W.B. Quayle^{164a,164b},
M. Queitsch-Maitland⁸⁴, D. Quilty⁵³, S. Raddum¹¹⁹, V. Radeka²⁵, V. Radescu⁴², S.K. Radhakrishnan¹⁴⁸,
P. Radloff¹¹⁶, P. Rados⁸⁸, F. Ragusa^{91a,91b}, G. Rahal¹⁷⁸, S. Rajagopalan²⁵, M. Rammensee³⁰,
C. Rangel-Smith¹⁶⁶, F. Rauscher¹⁰⁰, S. Rave⁸³, T. Ravenscroft⁵³, M. Raymond³⁰, A.L. Read¹¹⁹,
N.P. Readoff⁷⁴, D.M. Rebuzzi^{121a,121b}, A. Redelbach¹⁷⁴, G. Redlinger²⁵, R. Reece¹³⁷, K. Reeves⁴¹,
L. Rehnisch¹⁶, J. Reichert¹²², H. Reisin²⁷, M. Relich¹⁶³, C. Rembser³⁰, H. Ren^{33a}, A. Renaud¹¹⁷,
M. Rescigno^{132a}, S. Resconi^{91a}, O.L. Rezanova^{109,c}, P. Reznicek¹²⁹, R. Rezvani⁹⁵, R. Richter¹⁰¹,
S. Richter⁷⁸, E. Richter-Was^{38b}, O. Ricken²¹, M. Ridel⁸⁰, P. Rieck¹⁶, C.J. Riegel¹⁷⁵, J. Rieger⁵⁴, O. Rifki¹¹³,
M. Rijssenbeek¹⁴⁸, A. Rimoldi^{121a,121b}, L. Rinaldi^{20a}, B. Ristić⁴⁹, E. Ritsch³⁰, I. Riu¹², F. Rizatdinova¹¹⁴,
E. Rizvi⁷⁶, S.H. Robertson^{87,k}, A. Robichaud-Veronneau⁸⁷, D. Robinson²⁸, J.E.M. Robinson⁴²,
A. Robson⁵³, C. Roda^{124a,124b}, S. Roe³⁰, O. Røhne¹¹⁹, S. Rolli¹⁶¹, A. Romaniouk⁹⁸, M. Romano^{20a,20b},
S.M. Romano Saez³⁴, E. Romero Adam¹⁶⁷, N. Rompotis¹³⁸, M. Ronzani⁴⁸, L. Roos⁸⁰, E. Ros¹⁶⁷,
S. Rosati^{132a}, K. Rosbach⁴⁸, P. Rose¹³⁷, P.L. Rosendahl¹⁴, O. Rosenthal¹⁴¹, V. Rossetti^{146a,146b},
E. Rossi^{104a,104b}, L.P. Rossi^{50a}, J.H.N. Rosten²⁸, R. Rosten¹³⁸, M. Rotaru^{26a}, I. Roth¹⁷², J. Rothberg¹³⁸,
D. Rousseau¹¹⁷, C.R. Royon¹³⁶, A. Rozanov⁸⁵, Y. Rozen¹⁵², X. Ruan^{145c}, F. Rubbo¹⁴³, I. Rubinskiy⁴²,
V.I. Rud⁹⁹, C. Rudolph⁴⁴, M.S. Rudolph¹⁵⁸, F. Rühr⁴⁸, A. Ruiz-Martinez³⁰, Z. Rurikova⁴⁸,
N.A. Rusakovich⁶⁵, A. Ruschke¹⁰⁰, H.L. Russell¹³⁸, J.P. Rutherford⁷, N. Ruthmann⁴⁸, Y.F. Ryabov¹²³,
M. Rybar¹⁶⁵, G. Rybkin¹¹⁷, N.C. Ryder¹²⁰, A.F. Saavedra¹⁵⁰, G. Sabato¹⁰⁷, S. Sacerdoti²⁷, A. Saddique³,
H.F.W. Sadrozinski¹³⁷, R. Sadykov⁶⁵, F. Safai Tehrani^{132a}, M. Sahinsoy^{58a}, M. Saimpert¹³⁶, T. Saito¹⁵⁵,
H. Sakamoto¹⁵⁵, Y. Sakurai¹⁷¹, G. Salamanna^{134a,134b}, A. Salamon^{133a}, J.E. Salazar Loyola^{32b},
M. Saleem¹¹³, D. Salek¹⁰⁷, P.H. Sales De Bruin¹³⁸, D. Salihagic¹⁰¹, A. Salnikov¹⁴³, J. Salt¹⁶⁷,
D. Salvatore^{37a,37b}, F. Salvatore¹⁴⁹, A. Salvucci^{60a}, A. Salzburger³⁰, D. Sammel⁴⁸, D. Sampsonidis¹⁵⁴,
A. Sanchez^{104a,104b}, J. Sánchez¹⁶⁷, V. Sanchez Martinez¹⁶⁷, H. Sandaker¹¹⁹, R.L. Sandbach⁷⁶,
H.G. Sander⁸³, M.P. Sanders¹⁰⁰, M. Sandhoff¹⁷⁵, C. Sandoval¹⁶², R. Sandstroem¹⁰¹, D.P.C. Sankey¹³¹,
M. Sannino^{50a,50b}, A. Sansoni⁴⁷, C. Santoni³⁴, R. Santonico^{133a,133b}, H. Santos^{126a}, I. Santoyo Castillo¹⁴⁹,
K. Sapp¹²⁵, A. Saponov⁶⁵, J.G. Saraiva^{126a,126d}, B. Sarrazin²¹, O. Sasaki⁶⁶, Y. Sasaki¹⁵⁵, K. Sato¹⁶⁰,
G. Sauvage^{5,*}, E. Sauvan⁵, G. Savage⁷⁷, P. Savard^{158,d}, C. Sawyer¹³¹, L. Sawyer^{79,n}, J. Saxon³¹,
C. Sbarra^{20a}, A. Sbrizzi^{20a,20b}, T. Scanlon⁷⁸, D.A. Scannicchio¹⁶³, M. Scarcella¹⁵⁰, V. Scarfone^{37a,37b},
J. Schaarschmidt¹⁷², P. Schacht¹⁰¹, D. Schaefer³⁰, R. Schaefer⁴², J. Schaeffer⁸³, S. Schaepe²¹,
S. Schaetzel^{58b}, U. Schäfer⁸³, A.C. Schaffer¹¹⁷, D. Schaile¹⁰⁰, R.D. Schamberger¹⁴⁸, V. Scharf^{58a},
V.A. Schegelsky¹²³, D. Scheirich¹²⁹, M. Schernau¹⁶³, C. Schiavi^{50a,50b}, C. Schillo⁴⁸, M. Schioppa^{37a,37b},
S. Schlenker³⁰, K. Schmieden³⁰, C. Schmitt⁸³, S. Schmitt^{58b}, S. Schmitt⁴², B. Schneider^{159a},
Y.J. Schnellbach⁷⁴, U. Schnoor⁴⁴, L. Schoeffel¹³⁶, A. Schoening^{58b}, B.D. Schoenrock⁹⁰, E. Schopf²¹,
A.L.S. Schorlemmer⁵⁴, M. Schott⁸³, D. Schouten^{159a}, J. Schovancova⁸, S. Schramm⁴⁹, M. Schreyer¹⁷⁴,
C. Schroeder⁸³, N. Schuh⁸³, M.J. Schultens²¹, H.-C. Schultz-Coulon^{58a}, H. Schulz¹⁶, M. Schumacher⁴⁸,
B.A. Schumm¹³⁷, Ph. Schune¹³⁶, C. Schwanenberger⁸⁴, A. Schwartzman¹⁴³, T.A. Schwarz⁸⁹,
Ph. Schwegler¹⁰¹, H. Schweiger⁸⁴, Ph. Schwemling¹³⁶, R. Schwienhorst⁹⁰, J. Schwindling¹³⁶,
T. Schwindt²¹, F.G. Sciacca¹⁷, E. Scifo¹¹⁷, G. Sciolla²³, F. Scuri^{124a,124b}, F. Scutti²¹, J. Searcy⁸⁹,
G. Sedov⁴², E. Sedykh¹²³, P. Seema²¹, S.C. Seidel¹⁰⁵, A. Seiden¹³⁷, F. Seifert¹²⁸, J.M. Seixas^{24a},
G. Sekhniaidze^{104a}, K. Sekhon⁸⁹, S.J. Sekula⁴⁰, D.M. Seliverstov^{123,*}, N. Semprini-Cesari^{20a,20b},
C. Serfon³⁰, L. Serin¹¹⁷, L. Serkin^{164a,164b}, T. Serre⁸⁵, M. Sessa^{134a,134b}, R. Seuster^{159a}, H. Severini¹¹³,
T. Sfiligoi⁷⁵, F. Sforza³⁰, A. Sfyrla³⁰, E. Shabalina⁵⁴, M. Shamim¹¹⁶, L.Y. Shan^{33a}, R. Shang¹⁶⁵,
J.T. Shank²², M. Shapiro¹⁵, P.B. Shatalov⁹⁷, K. Shaw^{164a,164b}, S.M. Shaw⁸⁴, A. Shcherbakova^{146a,146b},
C.Y. Shehu¹⁴⁹, P. Sherwood⁷⁸, L. Shi^{151,af}, S. Shimizu⁶⁷, C.O. Shimmin¹⁶³, M. Shimojima¹⁰²,
M. Shiyakova⁶⁵, A. Shmeleva⁹⁶, D. Shoaleh Saadi⁹⁵, M.J. Shochet³¹, S. Shojaii^{91a,91b}, S. Shrestha¹¹¹,
E. Shulga⁹⁸, M.A. Shupe⁷, S. Shushkevich⁴², P. Sicho¹²⁷, P.E. Sidebo¹⁴⁷, O. Sidiropoulou¹⁷⁴,
D. Sidorov¹¹⁴, A. Sidoti^{20a,20b}, F. Siegert⁴⁴, Dj. Sijacki¹³, J. Silva^{126a,126d}, Y. Silver¹⁵³, S.B. Silverstein^{146a},
V. Simak¹²⁸, O. Simard⁵, Lj. Simic¹³, S. Simion¹¹⁷, E. Simioni⁸³, B. Simmons⁷⁸, D. Simon³⁴,
P. Sinervo¹⁵⁸, N.B. Sinev¹¹⁶, M. Sioli^{20a,20b}, G. Siragusa¹⁷⁴, A.N. Sisakyan^{65,*}, S.Yu. Sivoklov⁹⁹,
J. Sjölin^{146a,146b}, T.B. Sjsursen¹⁴, M.B. Skinner⁷², H.P. Skottowe⁵⁷, P. Skubic¹¹³, M. Slater¹⁸,
T. Slavicek¹²⁸, M. Slawinska¹⁰⁷, K. Sliwa¹⁶¹, V. Smakhtin¹⁷², B.H. Smart⁴⁶, L. Smestad¹⁴,

S.Yu. Smirnov⁹⁸, Y. Smirnov⁹⁸, L.N. Smirnova^{99,ag}, O. Smirnova⁸¹, M.N.K. Smith³⁵, R.W. Smith³⁵, M. Smizanska⁷², K. Smolek¹²⁸, A.A. Snesarev⁹⁶, G. Snidero⁷⁶, S. Snyder²⁵, R. Sobie^{169,k}, F. Socher⁴⁴, A. Soffer¹⁵³, D.A. Soh^{151,af}, G. Sokhrannyi⁷⁵, C.A. Solans³⁰, M. Solar¹²⁸, J. Solc¹²⁸, E.Yu. Soldatov⁹⁸, U. Soldevila¹⁶⁷, A.A. Solodkov¹³⁰, A. Soloshenko⁶⁵, O.V. Solovyanov¹³⁰, V. Solovyev¹²³, P. Sommer⁴⁸, H.Y. Song^{33b}, N. Soni¹, A. Sood¹⁵, A. Sopczak¹²⁸, B. Sopko¹²⁸, V. Sopko¹²⁸, V. Sorin¹², D. Sosa^{58b}, M. Sosebee⁸, C.L. Sotiropoulou^{124a,124b}, R. Soualah^{164a,164c}, A.M. Soukharev^{109,c}, D. South⁴², B.C. Sowden⁷⁷, S. Spagnolo^{73a,73b}, M. Spalla^{124a,124b}, M. Spangenberg¹⁷⁰, F. Spanò⁷⁷, W.R. Spearman⁵⁷, D. Sperlich¹⁶, F. Spettel¹⁰¹, R. Spighi^{20a}, G. Spigo³⁰, L.A. Spiller⁸⁸, M. Spousta¹²⁹, T. Spreitzer¹⁵⁸, R.D. St. Denis^{53,*}, A. Stabile^{91a}, S. Staerz⁴⁴, J. Stahlman¹²², R. Stamen^{58a}, S. Stamm¹⁶, E. Stanecka³⁹, C. Stancu^{134a}, M. Stancu-Bellu⁴², M.M. Stanitzki⁴², S. Stapnes¹¹⁹, E.A. Starchenko¹³⁰, J. Stark⁵⁵, P. Staroba¹²⁷, P. Starovoitov^{58a}, R. Staszewski³⁹, P. Steinberg²⁵, B. Stelzer¹⁴², H.J. Stelzer³⁰, O. Stelzer-Chilton^{159a}, H. Stenzel⁵², G.A. Stewart⁵³, J.A. Stillings²¹, M.C. Stockton⁸⁷, M. Stoebe⁸⁷, G. Stoicea^{26a}, P. Stolte⁵⁴, S. Stonjek¹⁰¹, A.R. Stradling⁸, A. Straessner⁴⁴, M.E. Stramaglia¹⁷, J. Strandberg¹⁴⁷, S. Strandberg^{146a,146b}, A. Strandlie¹¹⁹, E. Strauss¹⁴³, M. Strauss¹¹³, P. Strizenec^{144b}, R. Ströhmer¹⁷⁴, D.M. Strom¹¹⁶, R. Stroynowski⁴⁰, A. Strubig¹⁰⁶, S.A. Stucci¹⁷, B. Stugu¹⁴, N.A. Styles⁴², D. Su¹⁴³, J. Su¹²⁵, R. Subramaniam⁷⁹, A. Succurro¹², Y. Sugaya¹¹⁸, M. Suk¹²⁸, V.V. Sulin⁹⁶, S. Sultansoy^{4c}, T. Sumida⁶⁸, S. Sun⁵⁷, X. Sun^{33a}, J.E. Sundermann⁴⁸, K. Suruliz¹⁴⁹, G. Susinno^{37a,37b}, M.R. Sutton¹⁴⁹, S. Suzuki⁶⁶, M. Svatos¹²⁷, M. Swiatkowski¹⁴³, I. Sykora^{144a}, T. Sykora¹²⁹, D. Ta⁴⁸, C. Taccini^{134a,134b}, K. Tackmann⁴², J. Taenzer¹⁵⁸, A. Taffard¹⁶³, R. Tafiout^{159a}, N. Taiblum¹⁵³, H. Takai²⁵, R. Takashima⁶⁹, H. Takeda⁶⁷, T. Takeshita¹⁴⁰, Y. Takubo⁶⁶, M. Talby⁸⁵, A.A. Talyshev^{109,c}, J.Y.C. Tam¹⁷⁴, K.G. Tan⁸⁸, J. Tanaka¹⁵⁵, R. Tanaka¹¹⁷, S. Tanaka⁶⁶, B.B. Tannenwald¹¹¹, N. Tannoury²¹, S. Tapprogge⁸³, S. Tarem¹⁵², F. Tarrade²⁹, G.F. Tartarelli^{91a}, P. Tas¹²⁹, M. Tasevsky¹²⁷, T. Tashiro⁶⁸, E. Tassi^{37a,37b}, A. Tavares Delgado^{126a,126b}, Y. Tayalati^{135d}, F.E. Taylor⁹⁴, G.N. Taylor⁸⁸, P.T.E. Taylor⁸⁸, W. Taylor^{159b}, F.A. Teischinger³⁰, M. Teixeira Dias Castanheira⁷⁶, P. Teixeira-Dias⁷⁷, K.K. Temming⁴⁸, D. Temple¹⁴², H. Ten Kate³⁰, P.K. Teng¹⁵¹, J.J. Teoh¹¹⁸, F. Tepel¹⁷⁵, S. Terada⁶⁶, K. Terashi¹⁵⁵, J. Terron⁸², S. Terzo¹⁰¹, M. Testa⁴⁷, R.J. Teuscher^{158,k}, T. Theveneaux-Pelzer³⁴, J.P. Thomas¹⁸, J. Thomas-Wilsker⁷⁷, E.N. Thompson³⁵, P.D. Thompson¹⁸, R.J. Thompson⁸⁴, A.S. Thompson⁵³, L.A. Thomsen¹⁷⁶, E. Thomson¹²², M. Thomson²⁸, R.P. Thun^{89,*}, M.J. Tibbetts¹⁵, R.E. Ticse Torres⁸⁵, V.O. Tikhomirov^{96,ah}, Yu.A. Tikhonov^{109,c}, S. Timoshenko⁹⁸, E. Tiouchichine⁸⁵, P. Tipton¹⁷⁶, S. Tisserant⁸⁵, K. Todome¹⁵⁷, T. Todorov^{5,*}, S. Todorova-Nova¹²⁹, J. Tojo⁷⁰, S. Tokár^{144a}, K. Tokushuku⁶⁶, K. Tollefson⁹⁰, E. Tolley⁵⁷, L. Tomlinson⁸⁴, M. Tomoto¹⁰³, L. Tompkins^{143,ai}, K. Toms¹⁰⁵, E. Torrence¹¹⁶, H. Torres¹⁴², E. Torró Pastor¹³⁸, J. Toth^{85,aj}, F. Touchard⁸⁵, D.R. Tovey¹³⁹, T. Trefzger¹⁷⁴, L. Tremblet³⁰, A. Tricoli³⁰, I.M. Trigger^{159a}, S. Trincas-Duvold⁸⁰, M.F. Tripiana¹², W. Trischuk¹⁵⁸, B. Trocmé⁵⁵, C. Troncon^{91a}, M. Trottier-McDonald¹⁵, M. Trovatelli¹⁶⁹, P. True⁹⁰, L. Truong^{164a,164c}, M. Trzebinski³⁹, A. Trzupek³⁹, C. Tsarouchas³⁰, J.C-L. Tseng¹²⁰, P.V. Tsiarehsha⁹², D. Tsionou¹⁵⁴, G. Tsipolitis¹⁰, N. Tsirintanis⁹, S. Tsiskaridze¹², V. Tsiskaridze⁴⁸, E.G. Tskhadadze^{51a}, I.I. Tsukerman⁹⁷, V. Tsulaia¹⁵, S. Tsuno⁶⁶, D. Tsybychev¹⁴⁸, A. Tudorache^{26a}, V. Tudorache^{26a}, A.N. Tuna⁵⁷, S.A. Tuppiti^{20a,20b}, S. Turchikhin^{99,ag}, D. Turecek¹²⁸, R. Turra^{91a,91b}, A.J. Turvey⁴⁰, P.M. Tuts³⁵, A. Tykhonov⁴⁹, M. Tylmad^{146a,146b}, M. Tyndel¹³¹, I. Ueda¹⁵⁵, R. Ueno²⁹, M. Ughetto^{146a,146b}, M. Uglund¹⁴, F. Ukegawa¹⁶⁰, G. Unal³⁰, A. Undrus²⁵, G. Unel¹⁶³, F.C. Ungaro⁴⁸, Y. Unno⁶⁶, C. Unverdorben¹⁰⁰, J. Urban^{144b}, P. Urquijo⁸⁸, P. Urrejola⁸³, G. Usai⁸, A. Usanova⁶², L. Vacavant⁸⁵, V. Vacek¹²⁸, B. Vachon⁸⁷, C. Valderanis⁸³, N. Valencic¹⁰⁷, S. Valentinetti^{20a,20b}, A. Valero¹⁶⁷, L. Valery¹², S. Valkar¹²⁹, E. Valladolid Gallego¹⁶⁷, S. Vallecorsa⁴⁹, J.A. Valls Ferrer¹⁶⁷, W. Van Den Wollenberg¹⁰⁷, P.C. Van Der Deijl¹⁰⁷, R. van der Geer¹⁰⁷, H. van der Graaf¹⁰⁷, N. van Eldik¹⁵², P. van Gemmeren⁶, J. Van Nieuwkoop¹⁴², I. van Vulpen¹⁰⁷, M.C. van Woerden³⁰, M. Vanadia^{132a,132b}, W. Vandelli³⁰, R. Vanguri¹²², A. Vaniachine⁶, F. Vannucci⁸⁰, G. Vardanyan¹⁷⁷, R. Vari^{132a}, E.W. Varnes⁷, T. Varol⁴⁰, D. Varouchas⁸⁰, A. Vartapetian⁸, K.E. Varvell¹⁵⁰, F. Vazeille³⁴, T. Vazquez Schroeder⁸⁷, J. Veatch⁷, L.M. Veloce¹⁵⁸, F. Veloso^{126a,126c}, T. Velz²¹, S. Veneziano^{132a}, A. Ventura^{73a,73b}, D. Ventura⁸⁶, M. Venturi¹⁶⁹, N. Venturi¹⁵⁸, A. Venturini²³, V. Vercesi^{121a}, M. Verducci^{132a,132b}, W. Verkerke¹⁰⁷, J.C. Vermeulen¹⁰⁷, A. Vest⁴⁴, M.C. Vetterli^{142,d}, O. Viazlo⁸¹, I. Vichou¹⁶⁵, T. Vickey¹³⁹, O.E. Vickey Boeriu¹³⁹, G.H.A. Viehhauser¹²⁰, S. Viel¹⁵, R. Vigne⁶², M. Villa^{20a,20b}, M. Villaplana Perez^{91a,91b}, E. Vilucchi⁴⁷, M.G. Vinciter²⁹, V.B. Vinogradov⁶⁵,

I. Vivarelli¹⁴⁹, F. Vives Vaque³, S. Vlachos¹⁰, D. Vladoiu¹⁰⁰, M. Vlasak¹²⁸, M. Vogel^{32a}, P. Vokac¹²⁸, G. Volpi^{124a,124b}, M. Volpi⁸⁸, H. von der Schmitt¹⁰¹, H. von Radziewski⁴⁸, E. von Toerne²¹, V. Vorobel¹²⁹, K. Vorobev⁹⁸, M. Vos¹⁶⁷, R. Voss³⁰, J.H. Vosseveld⁷⁴, N. Vranjes¹³, M. Vranjes Milosavljevic¹³, V. Vrba¹²⁷, M. Vreeswijk¹⁰⁷, R. Vuillermet³⁰, I. Vukotic³¹, Z. Vykydal¹²⁸, P. Wagner²¹, W. Wagner¹⁷⁵, H. Wahlberg⁷¹, S. Wahrmond⁴⁴, J. Wakabayashi¹⁰³, J. Walder⁷², R. Walker¹⁰⁰, W. Walkowiak¹⁴¹, C. Wang¹⁵¹, F. Wang¹⁷³, H. Wang¹⁵, H. Wang⁴⁰, J. Wang⁴², J. Wang^{33a}, K. Wang⁸⁷, R. Wang⁶, S.M. Wang¹⁵¹, T. Wang²¹, T. Wang³⁵, X. Wang¹⁷⁶, C. Wanotayaroj¹¹⁶, A. Warburton⁸⁷, C.P. Ward²⁸, D.R. Wardrope⁷⁸, A. Washbrook⁴⁶, C. Wasicki⁴², P.M. Watkins¹⁸, A.T. Watson¹⁸, I.J. Watson¹⁵⁰, M.F. Watson¹⁸, G. Watts¹³⁸, S. Watts⁸⁴, B.M. Waugh⁷⁸, S. Webb⁸⁴, M.S. Weber¹⁷, S.W. Weber¹⁷⁴, J.S. Webster³¹, A.R. Weidberg¹²⁰, B. Weinert⁶¹, J. Weingarten⁵⁴, C. Weiser⁴⁸, H. Weits¹⁰⁷, P.S. Wells³⁰, T. Wenaus²⁵, T. Wengler³⁰, S. Wenig³⁰, N. Wermes²¹, M. Werner⁴⁸, P. Werner³⁰, M. Wessels^{58a}, J. Wetter¹⁶¹, K. Whalen¹¹⁶, A.M. Wharton⁷², A. White⁸, M.J. White¹, R. White^{32b}, S. White^{124a,124b}, D. Whiteson¹⁶³, F.J. Wickens¹³¹, W. Wiedenmann¹⁷³, M. Wielers¹³¹, P. Wienemann²¹, C. Wiglesworth³⁶, L.A.M. Wiik-Fuchs²¹, A. Wildauer¹⁰¹, H.G. Wilkens³⁰, H.H. Williams¹²², S. Williams¹⁰⁷, C. Willis⁹⁰, S. Willocq⁸⁶, A. Wilson⁸⁹, J.A. Wilson¹⁸, I. Wingerter-Seez⁵, F. Winklmeier¹¹⁶, B.T. Winter²¹, M. Wittgen¹⁴³, J. Wittkowski¹⁰⁰, S.J. Wollstadt⁸³, M.W. Wolter³⁹, H. Wolters^{126a,126c}, B.K. Wosiek³⁹, J. Wotschack³⁰, M.J. Woudstra⁸⁴, K.W. Wozniak³⁹, M. Wu⁵⁵, M. Wu³¹, S.L. Wu¹⁷³, X. Wu⁴⁹, Y. Wu⁸⁹, T.R. Wyatt⁸⁴, B.M. Wynne⁴⁶, S. Xella³⁶, D. Xu^{33a}, L. Xu²⁵, B. Yabsley¹⁵⁰, S. Yacoob^{145a}, R. Yakabe⁶⁷, M. Yamada⁶⁶, D. Yamaguchi¹⁵⁷, Y. Yamaguchi¹¹⁸, A. Yamamoto⁶⁶, S. Yamamoto¹⁵⁵, T. Yamanaka¹⁵⁵, K. Yamauchi¹⁰³, Y. Yamazaki⁶⁷, Z. Yan²², H. Yang^{33e}, H. Yang¹⁷³, Y. Yang¹⁵¹, W.-M. Yao¹⁵, Y. Yasu⁶⁶, E. Yatsenko⁵, K.H. Yau Wong²¹, J. Ye⁴⁰, S. Ye²⁵, I. Yeletsikh⁶⁵, A.L. Yen⁵⁷, E. Yildirim⁴², K. Yorita¹⁷¹, R. Yoshida⁶, K. Yoshihara¹²², C. Young¹⁴³, C.J.S. Young³⁰, S. Youssef²², D.R. Yu¹⁵, J. Yu⁸, J.M. Yu⁸⁹, J. Yu¹¹⁴, L. Yuan⁶⁷, S.P.Y. Yuen²¹, A. Yurkewicz¹⁰⁸, I. Yusuff^{28,ak}, B. Zabinski³⁹, R. Zaidan⁶³, A.M. Zaitsev^{130,ab}, J. Zalieckas¹⁴, A. Zaman¹⁴⁸, S. Zambito⁵⁷, L. Zanello^{132a,132b}, D. Zanzi⁸⁸, C. Zeitnitz¹⁷⁵, M. Zeman¹²⁸, A. Zemla^{38a}, Q. Zeng¹⁴³, K. Zengel²³, O. Zenin¹³⁰, T. Ženiš^{144a}, D. Zerwas¹¹⁷, D. Zhang⁸⁹, F. Zhang¹⁷³, H. Zhang^{33c}, J. Zhang⁶, L. Zhang⁴⁸, R. Zhang^{33b}, X. Zhang^{33d}, Z. Zhang¹¹⁷, X. Zhao⁴⁰, Y. Zhao^{33d,117}, Z. Zhao^{33b}, A. Zhemchugov⁶⁵, J. Zhong¹²⁰, B. Zhou⁸⁹, C. Zhou⁴⁵, L. Zhou³⁵, L. Zhou⁴⁰, M. Zhou¹⁴⁸, N. Zhou^{33f}, C.G. Zhu^{33d}, H. Zhu^{33a}, J. Zhu⁸⁹, Y. Zhu^{33b}, X. Zhuang^{33a}, K. Zhukov⁹⁶, A. Zibell¹⁷⁴, D. Zieminska⁶¹, N.I. Zimine⁶⁵, C. Zimmermann⁸³, S. Zimmermann⁴⁸, Z. Zinonos⁵⁴, M. Zinser⁸³, M. Ziolkowski¹⁴¹, L. Živković¹³, G. Zobernig¹⁷³, A. Zoccoli^{20a,20b}, M. zur Nedden¹⁶, G. Zurzolo^{104a,104b}, L. Zwalinski³⁰

¹ Department of Physics, University of Adelaide, Adelaide, Australia

² Physics Department, SUNY Albany, Albany, NY, United States

³ Department of Physics, University of Alberta, Edmonton, AB, Canada

⁴ (a) Department of Physics, Ankara University, Ankara; (b) Istanbul Aydin University, Istanbul; (c) Division of Physics, TOBB University of Economics and Technology, Ankara, Turkey

⁵ LAPP, CNRS/IN2P3 and Université Savoie Mont Blanc, Annecy-le-Vieux, France

⁶ High Energy Physics Division, Argonne National Laboratory, Argonne, IL, United States

⁷ Department of Physics, University of Arizona, Tucson, AZ, United States

⁸ Department of Physics, The University of Texas at Arlington, Arlington, TX, United States

⁹ Physics Department, University of Athens, Athens, Greece

¹⁰ Physics Department, National Technical University of Athens, Zografou, Greece

¹¹ Institute of Physics, Azerbaijan Academy of Sciences, Baku, Azerbaijan

¹² Institut de Física d'Altes Energies and Departament de Física de la Universitat Autònoma de Barcelona, Barcelona, Spain

¹³ Institute of Physics, University of Belgrade, Belgrade, Serbia

¹⁴ Department for Physics and Technology, University of Bergen, Bergen, Norway

¹⁵ Physics Division, Lawrence Berkeley National Laboratory and University of California, Berkeley, CA, United States

¹⁶ Department of Physics, Humboldt University, Berlin, Germany

¹⁷ Albert Einstein Center for Fundamental Physics and Laboratory for High Energy Physics, University of Bern, Bern, Switzerland

¹⁸ School of Physics and Astronomy, University of Birmingham, Birmingham, United Kingdom

¹⁹ (a) Department of Physics, Bogazici University, Istanbul; (b) Department of Physics Engineering, Gaziantep University, Gaziantep; (c) Department of Physics, Dogus University, Istanbul, Turkey

²⁰ (a) INFN Sezione di Bologna; (b) Dipartimento di Fisica e Astronomia, Università di Bologna, Bologna, Italy

²¹ Physikalisches Institut, University of Bonn, Bonn, Germany

²² Department of Physics, Boston University, Boston, MA, United States

²³ Department of Physics, Brandeis University, Waltham, MA, United States

²⁴ (a) Universidade Federal do Rio De Janeiro COPPE/EE/IF, Rio de Janeiro; (b) Electrical Circuits Department, Federal University of Juiz de Fora (UFJF), Juiz de Fora; (c) Federal University of Sao Joao del Rei (UFSJ), Sao Joao del Rei; (d) Instituto de Física, Universidade de Sao Paulo, Sao Paulo, Brazil

²⁵ Physics Department, Brookhaven National Laboratory, Upton, NY, United States

²⁶ (a) National Institute of Physics and Nuclear Engineering, Bucharest; (b) National Institute for Research and Development of Isotopic and Molecular Technologies, Physics Department, Cluj Napoca; (c) University Politehnica Bucharest, Bucharest; (d) West University in Timisoara, Timisoara, Romania

²⁷ Departamento de Física, Universidad de Buenos Aires, Buenos Aires, Argentina

²⁸ Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom

- ²⁹ Department of Physics, Carleton University, Ottawa, ON, Canada
- ³⁰ CERN, Geneva, Switzerland
- ³¹ Enrico Fermi Institute, University of Chicago, Chicago, IL, United States
- ³² (a) Departamento de Física, Pontificia Universidad Católica de Chile, Santiago; (b) Departamento de Física, Universidad Técnica Federico Santa María, Valparaíso, Chile
- ³³ (a) Institute of High Energy Physics, Chinese Academy of Sciences, Beijing; (b) Department of Modern Physics, University of Science and Technology of China, Anhui; (c) Department of Physics, Nanjing University, Jiangsu; (d) School of Physics, Shandong University, Shandong; (e) Department of Physics and Astronomy, Shanghai Key Laboratory for Particle Physics and Cosmology, Shanghai Jiao Tong University, Shanghai; (f) Physics Department, Tsinghua University, Beijing 100084, China
- ³⁴ Laboratoire de Physique Corpusculaire, Clermont Université and Université Blaise Pascal and CNRS/IN2P3, Clermont-Ferrand, France
- ³⁵ Nevis Laboratory, Columbia University, Irvington, NY, United States
- ³⁶ Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark
- ³⁷ (a) INFN Gruppo Collegato di Cosenza, Laboratori Nazionali di Frascati; (b) Dipartimento di Fisica, Università della Calabria, Rende, Italy
- ³⁸ (a) AGH University of Science and Technology, Faculty of Physics and Applied Computer Science, Krakow; (b) Marian Smoluchowski Institute of Physics, Jagiellonian University, Krakow, Poland
- ³⁹ Institute of Nuclear Physics Polish Academy of Sciences, Krakow, Poland
- ⁴⁰ Physics Department, Southern Methodist University, Dallas, TX, United States
- ⁴¹ Physics Department, University of Texas at Dallas, Richardson, TX, United States
- ⁴² DESY, Hamburg and Zeuthen, Germany
- ⁴³ Institut für Experimentelle Physik IV, Technische Universität Dortmund, Dortmund, Germany
- ⁴⁴ Institut für Kern- und Teilchenphysik, Technische Universität Dresden, Dresden, Germany
- ⁴⁵ Department of Physics, Duke University, Durham, NC, United States
- ⁴⁶ SUPA – School of Physics and Astronomy, University of Edinburgh, Edinburgh, United Kingdom
- ⁴⁷ INFN Laboratori Nazionali di Frascati, Frascati, Italy
- ⁴⁸ Fakultät für Mathematik und Physik, Albert-Ludwigs-Universität, Freiburg, Germany
- ⁴⁹ Section de Physique, Université de Genève, Geneva, Switzerland
- ⁵⁰ (a) INFN Sezione di Genova; (b) Dipartimento di Fisica, Università di Genova, Genova, Italy
- ⁵¹ (a) E. Andronikashvili Institute of Physics, Iv. Javakishvili Tbilisi State University, Tbilisi; (b) High Energy Physics Institute, Tbilisi State University, Tbilisi, Georgia
- ⁵² II Physikalisches Institut, Justus-Liebig-Universität Giessen, Giessen, Germany
- ⁵³ SUPA – School of Physics and Astronomy, University of Glasgow, Glasgow, United Kingdom
- ⁵⁴ II Physikalisches Institut, Georg-August-Universität, Göttingen, Germany
- ⁵⁵ Laboratoire de Physique Subatomique et de Cosmologie, Université Grenoble-Alpes, CNRS/IN2P3, Grenoble, France
- ⁵⁶ Department of Physics, Hampton University, Hampton, VA, United States
- ⁵⁷ Laboratory for Particle Physics and Cosmology, Harvard University, Cambridge, MA, United States
- ⁵⁸ (a) Kirchhoff-Institut für Physik, Ruprecht-Karls-Universität Heidelberg, Heidelberg; (b) Physikalisches Institut, Ruprecht-Karls-Universität Heidelberg, Heidelberg; (c) ZITI Institut für technische Informatik, Ruprecht-Karls-Universität Heidelberg, Mannheim, Germany
- ⁵⁹ Faculty of Applied Information Science, Hiroshima Institute of Technology, Hiroshima, Japan
- ⁶⁰ (a) Department of Physics, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong; (b) Department of Physics, The University of Hong Kong, Hong Kong; (c) Department of Physics, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, China
- ⁶¹ Department of Physics, Indiana University, Bloomington, IN, United States
- ⁶² Institut für Astro- und Teilchenphysik, Leopold-Franzens-Universität, Innsbruck, Austria
- ⁶³ University of Iowa, Iowa City, IA, United States
- ⁶⁴ Department of Physics and Astronomy, Iowa State University, Ames, IA, United States
- ⁶⁵ Joint Institute for Nuclear Research, JINR Dubna, Dubna, Russia
- ⁶⁶ KEK, High Energy Accelerator Research Organization, Tsukuba, Japan
- ⁶⁷ Graduate School of Science, Kobe University, Kobe, Japan
- ⁶⁸ Faculty of Science, Kyoto University, Kyoto, Japan
- ⁶⁹ Kyoto University of Education, Kyoto, Japan
- ⁷⁰ Department of Physics, Kyushu University, Fukuoka, Japan
- ⁷¹ Instituto de Física La Plata, Universidad Nacional de La Plata and CONICET, La Plata, Argentina
- ⁷² Physics Department, Lancaster University, Lancaster, United Kingdom
- ⁷³ (a) INFN Sezione di Lecce; (b) Dipartimento di Matematica e Fisica, Università del Salento, Lecce, Italy
- ⁷⁴ Oliver Lodge Laboratory, University of Liverpool, Liverpool, United Kingdom
- ⁷⁵ Department of Physics, Jožef Stefan Institute and University of Ljubljana, Ljubljana, Slovenia
- ⁷⁶ School of Physics and Astronomy, Queen Mary University of London, London, United Kingdom
- ⁷⁷ Department of Physics, Royal Holloway University of London, Surrey, United Kingdom
- ⁷⁸ Department of Physics and Astronomy, University College London, London, United Kingdom
- ⁷⁹ Louisiana Tech University, Ruston, LA, United States
- ⁸⁰ Laboratoire de Physique Nucléaire et de Hautes Energies, UPMC and Université Paris-Diderot and CNRS/IN2P3, Paris, France
- ⁸¹ Fysiska institutionen, Lunds universitet, Lund, Sweden
- ⁸² Departamento de Física Teórica C-15, Universidad Autónoma de Madrid, Madrid, Spain
- ⁸³ Institut für Physik, Universität Mainz, Mainz, Germany
- ⁸⁴ School of Physics and Astronomy, University of Manchester, Manchester, United Kingdom
- ⁸⁵ CPPM, Aix-Marseille Université and CNRS/IN2P3, Marseille, France
- ⁸⁶ Department of Physics, University of Massachusetts, Amherst, MA, United States
- ⁸⁷ Department of Physics, McGill University, Montreal, QC, Canada
- ⁸⁸ School of Physics, University of Melbourne, Victoria, Australia
- ⁸⁹ Department of Physics, The University of Michigan, Ann Arbor, MI, United States
- ⁹⁰ Department of Physics and Astronomy, Michigan State University, East Lansing, MI, United States
- ⁹¹ (a) INFN Sezione di Milano; (b) Dipartimento di Fisica, Università di Milano, Milano, Italy
- ⁹² B.I. Stepanov Institute of Physics, National Academy of Sciences of Belarus, Minsk, Belarus
- ⁹³ National Scientific and Educational Centre for Particle and High Energy Physics, Minsk, Belarus
- ⁹⁴ Department of Physics, Massachusetts Institute of Technology, Cambridge, MA, United States
- ⁹⁵ Group of Particle Physics, University of Montreal, Montreal, QC, Canada
- ⁹⁶ P.N. Lebedev Institute of Physics, Academy of Sciences, Moscow, Russia
- ⁹⁷ Institute for Theoretical and Experimental Physics (ITEP), Moscow, Russia
- ⁹⁸ National Research Nuclear University MEPhI, Moscow, Russia
- ⁹⁹ D.V. Skobel'syn Institute of Nuclear Physics, M.V. Lomonosov Moscow State University, Moscow, Russia
- ¹⁰⁰ Fakultät für Physik, Ludwig-Maximilians-Universität München, München, Germany
- ¹⁰¹ Max-Planck-Institut für Physik (Werner-Heisenberg-Institut), München, Germany
- ¹⁰² Nagasaki Institute of Applied Science, Nagasaki, Japan

- ¹⁰³ Graduate School of Science and Kobayashi–Maskawa Institute, Nagoya University, Nagoya, Japan
- ¹⁰⁴ ^(a) INFN Sezione di Napoli; ^(b) Dipartimento di Fisica, Università di Napoli, Napoli, Italy
- ¹⁰⁵ Department of Physics and Astronomy, University of New Mexico, Albuquerque, NM, United States
- ¹⁰⁶ Institute for Mathematics, Astrophysics and Particle Physics, Radboud University Nijmegen/Nikhef, Nijmegen, Netherlands
- ¹⁰⁷ Nikhef National Institute for Subatomic Physics and University of Amsterdam, Amsterdam, Netherlands
- ¹⁰⁸ Department of Physics, Northern Illinois University, DeKalb, IL, United States
- ¹⁰⁹ Budker Institute of Nuclear Physics, SB RAS, Novosibirsk, Russia
- ¹¹⁰ Department of Physics, New York University, New York, NY, United States
- ¹¹¹ Ohio State University, Columbus, OH, United States
- ¹¹² Faculty of Science, Okayama University, Okayama, Japan
- ¹¹³ Homer L. Dodge Department of Physics and Astronomy, University of Oklahoma, Norman, OK, United States
- ¹¹⁴ Department of Physics, Oklahoma State University, Stillwater, OK, United States
- ¹¹⁵ Palacký University, RCPTM, Olomouc, Czech Republic
- ¹¹⁶ Center for High Energy Physics, University of Oregon, Eugene, OR, United States
- ¹¹⁷ LAL, Université Paris-Sud and CNRS/IN2P3, Orsay, France
- ¹¹⁸ Graduate School of Science, Osaka University, Osaka, Japan
- ¹¹⁹ Department of Physics, University of Oslo, Oslo, Norway
- ¹²⁰ Department of Physics, Oxford University, Oxford, United Kingdom
- ¹²¹ ^(a) INFN Sezione di Pavia; ^(b) Dipartimento di Fisica, Università di Pavia, Pavia, Italy
- ¹²² Department of Physics, University of Pennsylvania, Philadelphia, PA, United States
- ¹²³ National Research Centre “Kurchatov Institute” B.P. Konstantinov Petersburg Nuclear Physics Institute, St. Petersburg, Russia
- ¹²⁴ ^(a) INFN Sezione di Pisa; ^(b) Dipartimento di Fisica E. Fermi, Università di Pisa, Pisa, Italy
- ¹²⁵ Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, PA, United States
- ¹²⁶ ^(a) Laboratório de Instrumentação e Física Experimental de Partículas – LIP, Lisboa; ^(b) Faculdade de Ciências, Universidade de Lisboa, Lisboa; ^(c) Department of Physics, University of Coimbra, Coimbra; ^(d) Centro de Física Nuclear da Universidade de Lisboa, Lisboa; ^(e) Departamento de Física, Universidade do Minho, Braga; ^(f) Departamento de Física Teórica y del Cosmos and CAFPE, Universidad de Granada, Granada (Spain); ^(g) Dep Física and CEFITEC of Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Caparica, Portugal
- ¹²⁷ Institute of Physics, Academy of Sciences of the Czech Republic, Praha, Czech Republic
- ¹²⁸ Czech Technical University in Prague, Praha, Czech Republic
- ¹²⁹ Faculty of Mathematics and Physics, Charles University in Prague, Praha, Czech Republic
- ¹³⁰ State Research Center Institute for High Energy Physics, Protvino, Russia
- ¹³¹ Particle Physics Department, Rutherford Appleton Laboratory, Didcot, United Kingdom
- ¹³² ^(a) INFN Sezione di Roma; ^(b) Dipartimento di Fisica, Sapienza Università di Roma, Roma, Italy
- ¹³³ ^(a) INFN Sezione di Roma Tor Vergata; ^(b) Dipartimento di Fisica, Università di Roma Tor Vergata, Roma, Italy
- ¹³⁴ ^(a) INFN Sezione di Roma Tre; ^(b) Dipartimento di Matematica e Fisica, Università Roma Tre, Roma, Italy
- ¹³⁵ ^(a) Faculté des Sciences Ain Chock, Réseau Universitaire de Physique des Hautes Energies – Université Hassan II, Casablanca; ^(b) Centre National de l’Energie des Sciences Techniques Nucleaires, Rabat; ^(c) Faculté des Sciences Semlalia, Université Cadi Ayyad, LPHEA-Marrakech; ^(d) Faculté des Sciences, Université Mohamed Premier and LPTPM, Oujda; ^(e) Faculté des sciences, Université Mohammed V-Agdal, Rabat, Morocco
- ¹³⁶ DSM/IRFU (Institut de Recherches sur les Lois Fondamentales de l’Univers), CEA Saclay (Commissariat à l’Energie Atomique et aux Energies Alternatives), Gif-sur-Yvette, France
- ¹³⁷ Santa Cruz Institute for Particle Physics, University of California Santa Cruz, Santa Cruz, CA, United States
- ¹³⁸ Department of Physics, University of Washington, Seattle, WA, United States
- ¹³⁹ Department of Physics and Astronomy, University of Sheffield, Sheffield, United Kingdom
- ¹⁴⁰ Department of Physics, Shinshu University, Nagano, Japan
- ¹⁴¹ Fachbereich Physik, Universität Siegen, Siegen, Germany
- ¹⁴² Department of Physics, Simon Fraser University, Burnaby, BC, Canada
- ¹⁴³ SLAC National Accelerator Laboratory, Stanford, CA, United States
- ¹⁴⁴ ^(a) Faculty of Mathematics, Physics & Informatics, Comenius University, Bratislava; ^(b) Department of Subnuclear Physics, Institute of Experimental Physics of the Slovak Academy of Sciences, Kosice, Slovak Republic
- ¹⁴⁵ ^(a) Department of Physics, University of Cape Town, Cape Town; ^(b) Department of Physics, University of Johannesburg, Johannesburg; ^(c) School of Physics, University of the Witwatersrand, Johannesburg, South Africa
- ¹⁴⁶ ^(a) Department of Physics, Stockholm University; ^(b) The Oskar Klein Centre, Stockholm, Sweden
- ¹⁴⁷ Physics Department, Royal Institute of Technology, Stockholm, Sweden
- ¹⁴⁸ Departments of Physics & Astronomy and Chemistry, Stony Brook University, Stony Brook, NY, United States
- ¹⁴⁹ Department of Physics and Astronomy, University of Sussex, Brighton, United Kingdom
- ¹⁵⁰ School of Physics, University of Sydney, Sydney, Australia
- ¹⁵¹ Institute of Physics, Academia Sinica, Taipei, Taiwan
- ¹⁵² Department of Physics, Technion: Israel Institute of Technology, Haifa, Israel
- ¹⁵³ Raymond and Beverly Sackler School of Physics and Astronomy, Tel Aviv University, Tel Aviv, Israel
- ¹⁵⁴ Department of Physics, Aristotle University of Thessaloniki, Thessaloniki, Greece
- ¹⁵⁵ International Center for Elementary Particle Physics and Department of Physics, The University of Tokyo, Tokyo, Japan
- ¹⁵⁶ Graduate School of Science and Technology, Tokyo Metropolitan University, Tokyo, Japan
- ¹⁵⁷ Department of Physics, Tokyo Institute of Technology, Tokyo, Japan
- ¹⁵⁸ Department of Physics, University of Toronto, Toronto, ON, Canada
- ¹⁵⁹ ^(a) TRIUMF, Vancouver, BC; ^(b) Department of Physics and Astronomy, York University, Toronto, ON, Canada
- ¹⁶⁰ Faculty of Pure and Applied Sciences, University of Tsukuba, Tsukuba, Japan
- ¹⁶¹ Department of Physics and Astronomy, Tufts University, Medford, MA, United States
- ¹⁶² Centro de Investigaciones, Universidad Antonio Narino, Bogota, Colombia
- ¹⁶³ Department of Physics and Astronomy, University of California Irvine, Irvine, CA, United States
- ¹⁶⁴ ^(a) INFN Gruppo Collegato di Udine, Sezione di Trieste, Udine; ^(b) ICTP, Trieste; ^(c) Dipartimento di Chimica, Fisica e Ambiente, Università di Udine, Udine, Italy
- ¹⁶⁵ Department of Physics, University of Illinois, Urbana, IL, United States
- ¹⁶⁶ Department of Physics and Astronomy, University of Uppsala, Uppsala, Sweden
- ¹⁶⁷ Instituto de Física Corpuscular (IFIC) and Departamento de Física Atómica, Molecular y Nuclear and Departamento de Ingeniería Electrónica and Instituto de Microelectrónica de Barcelona (IMB-CNM), University of Valencia and CSIC, Valencia, Spain
- ¹⁶⁸ Department of Physics, University of British Columbia, Vancouver, BC, Canada
- ¹⁶⁹ Department of Physics and Astronomy, University of Victoria, Victoria, BC, Canada
- ¹⁷⁰ Department of Physics, University of Warwick, Coventry, United Kingdom
- ¹⁷¹ Waseda University, Tokyo, Japan
- ¹⁷² Department of Particle Physics, The Weizmann Institute of Science, Rehovot, Israel
- ¹⁷³ Department of Physics, University of Wisconsin, Madison, WI, United States
- ¹⁷⁴ Fakultät für Physik und Astronomie, Julius-Maximilians-Universität, Würzburg, Germany

¹⁷⁵ *Fachbereich C Physik, Bergische Universität Wuppertal, Wuppertal, Germany*

¹⁷⁶ *Department of Physics, Yale University, New Haven, CT, United States*

¹⁷⁷ *Yerevan Physics Institute, Yerevan, Armenia*

¹⁷⁸ *Centre de Calcul de l'Institut National de Physique Nucléaire et de Physique des Particules (IN2P3), Villeurbanne, France*

^a Also at Department of Physics, King's College London, London, United Kingdom.

^b Also at Institute of Physics, Azerbaijan Academy of Sciences, Baku, Azerbaijan.

^c Also at Novosibirsk State University, Novosibirsk, Russia.

^d Also at TRIUMF, Vancouver, BC, Canada.

^e Also at Department of Physics, California State University, Fresno, CA, United States.

^f Also at Department of Physics, University of Fribourg, Fribourg, Switzerland.

^g Also at Departamento de Física e Astronomia, Faculdade de Ciências, Universidade do Porto, Portugal.

^h Also at Tomsk State University, Tomsk, Russia.

ⁱ Also at CPPM, Aix-Marseille Université and CNRS/IN2P3, Marseille, France.

^j Also at Università di Napoli Parthenope, Napoli, Italy.

^k Also at Institute of Particle Physics (IPP), Canada.

^l Also at Particle Physics Department, Rutherford Appleton Laboratory, Didcot, United Kingdom.

^m Also at Department of Physics, St. Petersburg State Polytechnical University, St. Petersburg, Russia.

ⁿ Also at Louisiana Tech University, Ruston, LA, United States.

^o Also at Institutio Catalana de Recerca i Estudis Avancats, ICREA, Barcelona, Spain.

^p Also at Graduate School of Science, Osaka University, Osaka, Japan.

^q Also at Department of Physics, National Tsing Hua University, Taiwan.

^r Also at Department of Physics, The University of Texas at Austin, Austin, TX, United States.

^s Also at Institute of Theoretical Physics, Ilia State University, Tbilisi, Georgia.

^t Also at CERN, Geneva, Switzerland.

^u Also at Georgian Technical University (GTU), Tbilisi, Georgia.

^v Also at Manhattan College, New York, NY, United States.

^w Also at Hellenic Open University, Patras, Greece.

^x Also at Institute of Physics, Academia Sinica, Taipei, Taiwan.

^y Also at LAL, Université Paris-Sud and CNRS/IN2P3, Orsay, France.

^z Also at Academia Sinica Grid Computing, Institute of Physics, Academia Sinica, Taipei, Taiwan.

^{aa} Also at School of Physics, Shandong University, Shandong, China.

^{ab} Also at Moscow Institute of Physics and Technology State University, Dolgoprudny, Russia.

^{ac} Also at Section de Physique, Université de Genève, Geneva, Switzerland.

^{ad} Also at International School for Advanced Studies (SISSA), Trieste, Italy.

^{ae} Also at Department of Physics and Astronomy, University of South Carolina, Columbia, SC, United States.

^{af} Also at School of Physics and Engineering, Sun Yat-sen University, Guangzhou, China.

^{ag} Also at Faculty of Physics, M.V. Lomonosov Moscow State University, Moscow, Russia.

^{ah} Also at National Research Nuclear University MEPhI, Moscow, Russia.

^{ai} Also at Department of Physics, Stanford University, Stanford, CA, United States.

^{aj} Also at Institute for Particle and Nuclear Physics, Wigner Research Centre for Physics, Budapest, Hungary.

^{ak} Also at University of Malaya, Department of Physics, Kuala Lumpur, Malaysia.

* Deceased.